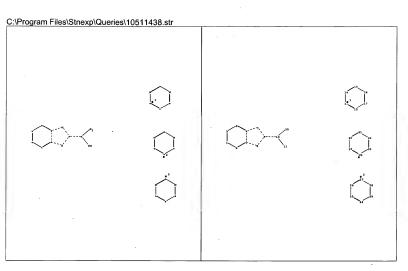
EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp		
L1	1926	((544/295) or (514/252.14)).CCLS.	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	OFF	2006/10/24 19:40		

	NPL Search Notes	Results
4.	TITLE-ABSTR-KEY(blood brain barrier) and TITLE-ABSTR-KEY(jnk and (inhibition or inhibit) and ischemia) [All Sources(- All Sciences -)]	3
3.	TITLE-ABSTR-KEY((expression or activity)) and TITLE-ABSTR-KEY(jnk and (inhibition or inhibit) and ischemia) [All Sources(- All Sciences -)]	88
2.	TITLE-ABSTR-KEY((expression or activity)) and TITLE-ABSTR-KEY(jnk and (inhibition or inhibit)) [All Sources(- All Sciences -)]	3033
1.	TITLE-ABSTR-KEY((expression or activity)) and TITLE-ABSTR-KEY(jnk) [All Sources(- All Sciences -)]	7878

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chain nodes : 10 11 35

10 11 30

ring nodes :

1 2 3 4 5 6 7 8 9 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29

chain bonds :

8-10 10-11 10-35

ring bonds :

ing bonds .

1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-9 7-8 8-9 12-13 12-17 13-14 14-15 15-16 16-17 18-19 18-23 19-20 20-21 21-22 22-23 24-25 24-29 25-26 26-27 27-28 28-29

exact/norm bonds :

4-5 4-7 5-9 7-8 8-9 8-10 10-35

exact bonds : 10-11

normalized bonds:

1-2 1-6 2-3 3-4 5-6 12-13 12-17 13-14 14-15 15-16 16-17 18-19 18-23 19-20 20-21 21-22

22-23 24-25 24-29 25-26 26-27 27-28 28-29

isolated ring systems:

containing 1: 12: 18: 24:

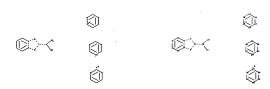
G1:[*1],[*2],[*3]

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLAS\$11:CLAS\$12:Atom 13:Atom

14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 35:CLASS

Uploading C:\Program Files\Stnexp\Queries\10168718.str



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chain nodes :
10 11 35
ring nodes :
1 2 3 4 5 6 7 8 9 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29
chain bonds :
8-10 10-11 10-35
ring bonds :
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-9 7-8 8-9 12-13 12-17 13-14 14-15 15-16
16-17 18-19 18-23 19-20 20-21 21-22 22-23 24-25 24-29 25-26 26-27 27-28
28-29
exact/norm bonds :
4-5 4-7 5-9 7-8 8-9 8-10 10-35
exact bonds :
10-11
normalized bonds :
1-2 1-6 2-3 3-4 5-6 12-13 12-17 13-14 14-15 15-16 16-17 18-19 18-23 19-20 20-21 21-22 22-23 24-25 24-29 25-26 26-27 27-28 28-29
isolated ring systems :
```

containing 1 : 12 : 18 : 24 :

G1:[*1],[*2],[*3]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20: Atom 21: Atom 22: Atom 23: Atom 24: Atom 25: Atom 26: Atom 27: Atom 28: Atom 29:Atom 35:CLASS

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s 11 sss sam

SAMPLE SEARCH INITIATED 14:19:34 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED -19 TO ITERATE

100.0% PROCESSED

19 ITERATIONS SEARCH TIME: 00.00.01

17 ANSWERS

587

FULL FILE PROJECTIONS: ONLINE **COMPLETE** **COMPLETE**

119 TO 641

PROJECTED ITERATIONS: BATCH PROJECTED ANSWERS: 93 TO

17 SEA SSS SAM L1

=> => s 11 sss fu1 FULL SEARCH INITIATED 14:20:49 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 278 TO ITERATE

100.0% PROCESSED 278 ITERATIONS

266 ANSWERS SEARCH TIME: 00.00.01

L3 266 SEA SSS FUL L1

=> => s 13

L4 16 L3

=> d 14 1-16 bib, ab, hitstr

10/511,438

L4 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2006:769183 CAPLUS

DN 145:181019

TI Use of inhibitors of jun N-terminal kinases to treat glaucoma

IN Fleenor, Debra L.; Pang, Iok-Hou

PA Alcon, Inc., USA

SO U.S. Pat. Appl. Publ., 14pp., Cont.-in-part of U.S. Ser. No. 259,566. CODEN: USXXCO

DT Patent

LA English

FAN. CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
PI US 2006172991	Al	20060803	US 2006-394893	20060331		
US 2006094753	A1	20060504	US 2005-259566	20051026		
PRAI US 2004-623755P	P	20041029				
US 2005-259566	A2	20051026				

AB Compns. and methods for lowering intraocular pressure (IOP) and/or providing neuroprotection are disclosed. The compns. and methods are particularly directed to the use inhibitors of Jun N-terminal kinases (JNK) to lower IOP and/or provide neuroprotection.

IT 861411-83-8

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(JNK kinase inhibitors for treatment of glaucoma)

RN 861411-83-8 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[2-(3-pyridinyl)ethyl]amino]-, (αZ)- (9CI) (CA INDEX NAME)

10/511.438

T.4 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2006:763978 CAPLUS

DN 145:159088

ΤТ Designing heterocyclic selective kinase inhibitors: from concept to new drug candidates IIA

Halazy, Serge

Serono Pharmaceutical Research Institute, Geneva, Switz. CS

SO ARKIVOC (Gainesville, FL, United States) (2006), (7), 496-508 CODEN: AGFUAR

URL: http://www.arkat-usa.org/ARKIVOC/JOURNAL CONTENT/manuscripts/2006/HL-1867GR%20as%20published%20mainmanuscript.pdfcastype

PB Arkat USA Inc.

DT Journal; (online computer file)

LA English

AB Kinases represent one of the most popular and promising target class in drug discovery. Success in finding new therapeutics will depend on the validation of the kinase chosen with respect to the disease of interest, and on the ability of chemists to design and synthesize inhibitors which are selective for this particular kinase. One of the most powerful validation tool for kinases is the Analog-Sensitive Kinase Allele (ASKA) technol., where chemists and biologists have engineered modified kinases and inhibitors by generating functionally active kinase mutants which are specifically inhibited by a chemical modified inhibitor, thus allowing to study specific responses in knock-in animals. The design of selective, ATP competitive kinase inhibitors has been successfully achieved by combining different technologies like computational chemical, structure-based design and combinatorial chemical as illustrated by the discovery of AS602801, a potent and selective JNK inhibitor with therapeutic potential in MS and fibrosis. The exploration of non ATP-competitive inhibitors is also very promising, as illustrated by the case of MEK inhibitors which show strong interest as anti-cancer agents. In the future, the rationale design of selective kinase inhibitors will move to the design of compds. that will induce a selective perturbation of cell regulation, where kinases play a critical role.

TТ 345987-15-7, AS601245 848344-36-5, AS 602801 RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(designing heterocyclic selective kinase inhibitors)

RN 345987-15-7 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(3-pyridinyl)ethyl]amino]-4pyrimidinyl] - (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{CN} & \text{N} \\ \hline & \text{CH} & \text{N} \\ \hline & \text{N} \\ \end{array} \text{NH-CH}_2\text{-CH}_2 \\ \hline & \text{N} \\ \end{array}$$

RN 848344-36-5 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-(4morpholinylmethyl)phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/511,438

- L4 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2006:506341 CAPLUS
- DN 145:95781
- TI Exploration of a Binding Mode of Benzothiazol-2-yl Acetonitrile Pyrimidine Core Based Derivatives as Potent c-Jun N-Terminal Kinase-3 Inhibitors and 3D-QSAR Analyses
- AU Sharma, Pooja; Ghoshal, Nanda
- CS Drug Design Development and Molecular Modeling Division, Indian Institute of Chemical Biology (CSIR), Kolkata, 700032, India
- SO Journal of Chemical Information and Modeling (2006), 46(4), 1763-1774 CODEN: JCISD8; ISSN: 1549-9596
- PB American Chemical Society
- DT Journal
- LA English
- C-Jun N-terminal kinase (JNK) is a therapeutic target for inhibitors which AB may provide clin. benefit in the pathogenesis of rheumatoid arthritis (RA) as well as in various apoptosis-related disorders. The benzothiazol-2-yl acetonitrile derivs., recently reported by Pascale et al. (J. Med. Chem. 2005, 48, 4596-4607), are the first generation JNK inhibitors of this class. To understand inhibitory mechanisms and elucidate pharmacophoric properties of these derivs. mol. docking and 3D-QSAR studies were performed on a set of 44 compds. Ligand Fit module of Cerius2 (4.9) was employed to locate the binding orientations of all the compds. within the JNK-3 ATP binding site. A good correlation (r2=0.810) between the calculated binding free energies (-PMF score) and the exptl. inhibitory activities suggests that the identified binding conformations of these potential inhibitors are reliable. Based on the binding conformations, robust and highly predictive 3D-QSAR models were developed with conventional r2 0.886 and 0.802, full cross-validation r2 0.980 and 0.788, and predictive r2 0.965 and 0.968 for MFA and MSA, resp. The interaction mode was demonstrated taking into consideration inhibitor conformation, hydrogen bonding, and electrostatic interaction. The 3D-QSAR model built in this study will provide clear guidelines for a novel inhibitor design based on the benzothiazole derivs. against JNK-3 for the treatment of inflammatory disorders.
- IT 861411-30-5 861411-33-8 861411-37-2 861411-38-3 861411-39-3 861411-40-6 861411-40-7 861411-45-2 861411-45-2 861411-45-2 861411-45-2 861411-45-2 861411-45-3 861411-51-0 861411-52-1 861411-52-1 861411-52-1 861411-52-1 861411-52-1 861411-53-2 861411-55-6 861411-55-6 861411-58-7 861411-69-8 861411-66-7 861411-67-8 861411-67-8 861411-67-8 861411-75-0 861411-75-0 861411-75-1 861
 - RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 - (QSAR and binding mode of benzothiazolyl acetonitrile pyrimidine core based derivs. as potent c-Jun N-terminal kinase-3 inhibitors)
- RN 861411-30-5 CAPLUS

895538-16-6 895538-17-7

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-chloro-, (αZ)- (9CI) (CA INDEX NAME) Double bond geometry as shown.

RN 861411-33-8 CAPLUS

CN 4-Pyrimidineacetonitrile, 2-chloro-α-[5-(trifluoromethyl)-2(3H)-benzothiazolylidene]-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

$$\begin{array}{c|c} & & CN \\ \hline & S \\ \hline & & NH \\ \hline & & & C1 \\ \end{array}$$

RN 861411-37-2 CAPLUS

CN 4-Pyrimidineacetonitrile, 2-amino- α -2(3H)-benzothiazolylidene-, (α Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-38-3 CAPLUS

CN 4-Pyrimidineacetonitrile, α -2(3H)-benzothiazolylidene-2-hydrazino-, (α Z)- (9CI) (CA INDEX NAME)

RN 861411-39-4 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-(methylamino)-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-40-7 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-(dimethylamino)-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-41-8 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-(1-piperazinyl)-, (αZ)- (9CI) (CA INDEX NAME)

RN

861411-42-9 CAPLUS 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-(4-methyl-1-piperazinyl)-, (α2)- (9CI) (CA INDEX NAME) CN

Double bond geometry as shown.

RN 861411-43-0 CAPLUS

CN 4-Pyrimidineacetonitrile, α -2(3H)-benzothiazolylidene-2-(4-morpholinyl)-, (α Z)- (9CI) (CA INDEX NAME)

- RN 861411-45-2 CAPLUS
- CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-(4-hydroxy-1-piperidinyl)-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

- RN 861411-46-3 CAPLUS
- CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[(2-(dimethylamino)ethyl]amino]-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-47-4 CAPLUS

CN 4-Pyrimidineacetonitrile, 2-[(2-aminoethyl)amino]-α-2(3H)-benzothiazolylidene-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-48-5 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[(2-methoxyethyl)amino]-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-49-6 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[(2-hydroxyethyl)amino]-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-51-0 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[2-(1-piperidinyl)ethyl]amino]-, (αZ)- (9CI) (CA INDEX NAME)

RN 861411-52-1 CAPLUS

CN 4-Pyrimidineacetonitrile, \(\alpha - 2 \) (3H) -benzothiazolylidene-2-\[\] (2-(4-morpholinyl)ethyl]amino]-, \(\alpha Z \)) - (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-53-2 CAPLUS

CN 4-Pyrimidineacetonitrile, $\alpha-2(3H)$ -benzothiazolylidene-2-[[3-(dimethylamino)propyl]amino]-, (αZ) - (9CI) (CA INDEX NAME)

RN 861411-54-3 CAPLUS

CN 4-Pyrimidineacetonitrile, 2-[(3-aminopropyl)amino]-α-2(3H)-benzothiazolylidene-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-55-4 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-((3-hydroxypropyl)amino]-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-56-5 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[3-(4-morpholinyl)propyl]amino]-, (αZ)- (9CI) (CA INDEX NAME)

RN 861411-57-6 CAPLUS CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[3-(4-methyl-1-piperazinyl)propyl]amino]-, (α2)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-58-7 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[3-(2-oxo-1-pyrrolidinyl)propyl]amino]-, (αZ)- (9CI) (CA INDEX NAME)

RN 861411-60-1 CAPLUS CN 4-Pyrimidineacetoni

4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[(phenylmethyl)amino]-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-61-2 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[(2-pyridinylmethyl)amino]-, (αZ)- (9CI) (CA INDEX NAME)

RN 861411-62-3 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[(3-pyridinylmethyl)amino]-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-63-4 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[(4-pyridinylmethyl)amino]-, (α2)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-66-7 CAPLUS

CN 4-Pyrimidineacetonitrile, α -2(3H)-benzothiazolylidene-2-[[2-(2-fluorophenyl)ethyl]amino]-, (α Z)- (9CI) (CA INDEX NAME)

RN 861411-67-8 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[2-(3-fluorophenyl)ethyl]amino]-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-73-6 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[2-(4-hydroxyphenyl)ethyl]amino]-, (αZ)- (9CI) (CA INDEX NAME)

RN 861411-74-7 CAPLUS

CN 4-Pyrimidineacetonitrile, α -2(3H)-benzothiazolylidene-2-[[2-(4-methoxyphenyl)ethyl]amino]-, (α Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-75-8 CAPLUS

CN 4-Pyrimidineacetonitrile, 2-[[2-(4-aminophenyl)ethyl]amino]-α-2(3H)-benzothiazolylidene-, (αZ)- (9CI) (CA INDEX NAME)

RN 861411-76-9 CAPLUS

CN Benzenesulfonamide, 4-[2-[[4-[(Z)-2(3H)-benzothiazolylidenecyanomethyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-77-0 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[2-(4-nitrophenyl)ethyl]amino]-, (αZ)- (9CI) (CA INDEX NAME)

RN 861411-78-1 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[2-(1H-indol-3-yl)ethyl]amino]-, (αΣ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-79-2 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[2-(1H-imidazol-4-yl)ethyl]amino]-, (αZ)- (9CI) (CA INDEX NAME)

RN .861411-80-5 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[2-(1-methyl-1H-imidazol-4-yl)ethyl]amino]-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-81-6 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[2-(1-methyl-1H-imidazol-2-yl)ethyl]amino]-, (αZ)- (9CI) (CA INDEX NAME)

RN 861411-82-7 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[2-(2-pyridinyl)ethyl]amino]-, (α2)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-83-8 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[2-(3-pyridinyl)ethyl]amino]-, (α2)- (9CI) (CA INDEX NAME)

RN 861411-84-9 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[2-(1H-1,2,4-triazol-1-yl)ethyl]amino]-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-85-0 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[3-(1H-imidazol-1-yl)propyl]amino]-, (αZ)- (9CI) (CA INDEX NAME)

RN 861411-86-1 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[3-(1H-pyrazol-1-yl)propyl]amino]-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 895538-16-6 CAPLUS

CN

4-Pyrimidineacetonitrile, α -2(3H)-benzothiazolylidene-2-[[3-(methylamino)propyl]amino]-, $(\alpha$ Z)- (9CI) (CA INDEX NAME)

RN 895538-17-7 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-6-bromo-2chloro-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RE.CNT 75 THERE ARE 75 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- 1.4 ANSWER 4 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2006:496089 CAPLUS
- DN 145:8158
- тΤ Preparation of benzothiazoles, their macrogol glyceride pharmaceutical formulations, and their therapeutic use
- IN Esposito, Pierandrea; Chicco, Daniela; Donati, Luca; Leonardi, Andrea; Bertero, Stefania; Gotteland, Jean-Pierre; Gaillard, Pascale; Jeanclaude-Etter, Isabelle; Grandolini, Simone; Maio, Mario
- Ares Trading S.A., Switz. PA PCT Int. Appl., 95 pp.
- SO CODEN: PIXXD2
- DТ Patent
- LA English

FAN.	CNT	1																
	PATENT NO.					KIND DA		DATE		APPLICATION NO.					DATE			
	,																	
PI	WO	O 2006053882			A2 20060526			WO 2005-EP56020						20051116				
	WO	2006053882			A3 20060908													
		W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	ΒZ,	CA,	CH,
			CN,	co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
			GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KM,	KN,	KP,	KR,
			ΚZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	LY,	MA,	MD,	MG,	MK,	MN,	MW,	MX,
			MZ,	NA,	NG,	NI,	NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	sc,	SD,	SE,
			SG,	sĸ,	SL,	SM,	SY,	ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UΖ,	vc,
			VN,	YU,	ZA,	ZM,	ZW											
		RW:	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,
			IS,	ΙT,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ВJ,
			CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG,	BW,	GH,
			GM,	ΚE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	ΤZ,	UG,	ZM,	ZW,	AM,	ΑZ,	BY,
			KG,	ΚZ,	MD,	RU,	ΤJ,	TM										
PRAI	EΡ	2004	-105	843		А		2004	1117									
	US	S 2004-628998P				P		2004	1118									

US 2004-628998P OS

20041118 MARPAT 145:8158

- AB The invention is related to macrogol glyceride pharmaceutical formulations containing benzothiazoles I [G = pyrimidinyl; L = alkoxy, NH2, 3-8 membered heterocycloalkyl containing ≥ 1 heteroatom selected from N. O. and S; R1 = H, NH2, CN, alk(en/yn)yl, etc.], as well as their tautomers, geometrical isomers, enantiomers, diastereomers, racemates, as well as their pharmaceutically acceptable salts. In particular, the invention is related to benzothiazole stearovl macrogol pharmaceutical formulations. method of preparation and use thereof. The invention is also related to the preparation of benzothiazoles I. Thus, benzothiazole II was prepared by reacting
- (1,3-benzothiazol-2-yl)acetonitrile with 2,4-dichloropyrimidine, followed by O-alkylation of 3-(2-hydroxyethyl)pyridine with the chloride intermediate. A stearoyl macrogol pharmaceutical formulation containing 20% weight/weight III dimesylate and 80% weight/weight Gelucire 50/13 (IV) was prepared I
- are useful for treating fibrosis, asthma, endometriosis, etc (no data).
- 888070-08-4P, (1,3-Benzothiazol-2-vl)[2-[2-(pyridin-3
 - vl)ethoxylpyrimidin-4-vllacetonitrile 888070-09-5P. (1,3-Benzothiazol-2-yl)[2-[(quinolin-6-yl)oxy]pyrimidin-4-yl]acetonitrile 888070-10-8P 888070-11-9P, (1,3-Benzothiazol-2-yl)[2-[[3-
 - [(4-methylpiperazin-1-y1)methyl]benzyl]oxy]pyrimidin-4-y1]acetonitrile 888070-12-0P 888070-13-1P, (1,3-Benzothiazol-2-yl)[2-
 - (hexyloxy)pyrimidin-4-yl]acetonitrile 888070-14-2P, (1,3-Benzothiazol-2-y1) [2-[[3-[(morpholin-4-y1)methyl]benzyl]oxy]pyrimidin-
 - 4-yl]acetonitrile 888070-15-3P, (1,3-Benzothiazol-2-yl)[2-[[3-

10/511.438

[(1H-imidazol-1-yl)methyl]benzyl]oxy]pyrimidin-4-yl]acetonitrile 888070-16-4P, (1,3-Benzothiazol-2-y1)[2-[[3-[(piperidin-1yl)methyl]benzyl]oxy]pyrimidin-4-yl]acetonitrile 888070-17-5P, (1,3-Benzothiazol-2-yl)[2-[[4-[(2,6-dimethylmorpholin-4yl)methyl]benzyl]oxy]pyrimidin-4-yl]acetonitrile 888070-18-6P 888070-19-7P 888070-20-0P, (1,3-Benzothiazol-2-yl)[2-[[4-[(benzylamino)methyl]benzyl]oxy]pyrimidin-4-yl]acetonitrile 888070-21-1P, (1,3-Benzothiazol-2-yl)[2-[[2-(morpholin-4vl)pyridin-4-yl]methoxy]pyrimidin-4-yl]acetonitrile 888070-22-2P , (1,3-Benzothiazol-2-yl)[2-[[2-(piperidin-1-yl)pyridin-4vl]methoxy]pyrimidin-4-yl]acetonitrile 888070-23-3P. (1,3-Benzothiazol-2-vl)[2-[2-(morpholin-4-vl)ethoxy]pyrimidin-4yl]acetonitrile 888070-24-4P 888070-25-5P, (1,3-Benzothiazol-2-vl)[2-[2-(dimethylamino)ethoxy]pyrimidin-4vllacetonitrile 888070-26-6P 888070-27-7P. (1,3-Benzothiazol-2-yl)[2-[3-(dimethylamino)propoxy]pyrimidin-4yl]acetonitrile 888070-28-8P, (1,3-Benzothiazol-2-yl)[2-[2-(4methylpiperazin-l-yl)ethoxy[pyrimidin-4-yl]acetonitrile 888070-29-9P, (1,3-Benzothiazol-2-yl)[2-[2-[2-(dimethylamino)ethoxy]ethoxy]pyrimidin-4-yl]acetonitrile 888070-30-2P 888070-31-3P 888070-32-4P 888070-33-5P 888070-34-6P RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (drug candidate; preparation of benzothiazoles, their macrogol glyceride pharmaceutical formulations, and their therapeutic use) 888070-08-4 CAPLUS

2-Benzothiazoleacetonitrile, \alpha -[2-[2-(3-pyridinyl)ethoxy]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 888070-09-5 CAPLUS

RN

CN

CN 2-Benzothiazoleacetonitrile, \alpha-[2-(6-quinolinyloxy)-4-pyrimidinyl]-(9CI) (CA INDEX NAME)

RN 888070-10-8 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[5-(4-morpholinvl)-3pyridinyllmethoxyl-4-pyrimidinyll- (9CI) (CA INDEX NAME)

RN 888070-11-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[3-[(4-methyl-1-piperaziny1)methyl]phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 888070-12-0 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-[(3,4-dihydro-2(1H)-isoquinolinyl)methyl]phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 888070-13-1 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-(hexyloxy)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 888070-14-2 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[3-(4-morpholinylmethyl)phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 888070-15-3 CAPLUS

CN 2-Benzothiazoleacetonitrile, \(\alpha - [2-[[3-(1\text{H-imidazol-1-} \) \] \) \(\text{ylmethyl} \) \(\text{phenyl} \] \(\text{methyl} \) \(\text{phenyl} \] \(\text{methyl} \) \(\text{Polynomial} \) \(\text{VAME} \) \(\text{VAME} \)

RN 888070-16-4 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[3-(1-piperidinylmethyl)phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\$$

RN 888070-17-5 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-[(2,6-dimethyl-4-morpholinyl)methyl]phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 888070-18-6 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[4-[[bis(2-methoxyethyl)amino]methyl]phenyl]methoxy]- (9CI) (CA INDEX NAME)

RN 888070-19-7 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[4-[[4-(1,1-dimethylethoxy)-1-piperidinyl]methyl]phenyl]methoxy]- (9CI) (CA INDEX NAME)

RN 888070-20-0 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-[[(phenylmethyl])amino]methyl]phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 888070-21-1 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(4-morpholinyl)-4-pyridinyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 888070-22-2 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(2-(1-piperidinyl)-4-pyridinyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 888070-23-3 CAPLUS

CN 2-Benzothiazoleacetonitrile, $\alpha-[2-[2-(4-morpholinyl)ethoxy]-4$ pyrimidinyl] - (9CI) (CA INDEX NAME)

RN 888070-24-4 CAPLUS

4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[(1,4-CN dimethyl-2-piperazinyl)methoxy]- (9CI) (CA INDEX NAME)

RN 888070-25-5 CAPLUS

2-Benzothiazoleacetonitrile, \alpha-[2-[2-(dimethylamino)ethoxy]-4-CN pyrimidinyl] - (9CI) (CA INDEX NAME)

RN

888070-26-6 CAPLUS Piperazine, 1-[4-[[[4-(2(3H)-benzothiazolylidenecyanomethyl)-2-CN pyrimidinyl]oxy]methyl]benzoyl]-4-methyl- (9CI) (CA INDEX NAME)

RN 888070-27-7 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[3-(dimethylamino)propoxy]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 888070-28-8 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[2-(4-methyl-1-piperazinyl)ethoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & CN & N & Me \\ \hline & CH & N & O-CH_2-CH_2-N & Me \end{array}$$

RN 888070-29-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, α -[2-[2-[2-(dimethylamino)ethoxy]ethoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 888070-30-2 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[2-(3-pyridinyl)ethoxy]-4-pyrimidinyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 888070-08-4 CMF C20 H15 N5 O S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 888070-31-3 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[5-(4-morpholiny1)-3pyridiny1]methoxy]-4-pyrimidiny1]-, methanesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 888070-10-8 CMF C23 H20 N6 O2 S

CM :

CRN 75-75-2 CMF C H4 O3 S

RN .888070-32-4 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[4-[[bis(2-methoxyethyl)amino]methyl]phenyl]methoxy]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM

CRN 888070-18-6 CMF C27 H29 N5 O3 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 888070-33-5 CAPLUS CN 4-Pyrimidineacetonit

4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[4-[[4-(1,1-dimethylethoxy)-1-piperidinyl]methyl]phethoxy]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 888070-19-7 CMF C30 H33 N5 O2 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 888070-34-6 CAPLUS CN 2-Benzothiazoleacet

2-Benzothiazoleacetonitrile, α -[2-[3-(dimethylamino)propoxy]-4-pyrimidinyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM

CRN 888070-27-7 CMF C18 H19 N5 O S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

IT 345986-38-1P, (1,3-Benzothiazol-2-yl)(2-chloro-4pyrimidinyl)acetonitrile

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of benzothiazoles, their macrogol glyceride pharmaceutical formulations, and their therapeutic use)

RN 345986-38-1 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-(2-chloro-4-pyrimidiny1)- (9CI) (CA INDEX NAME)

IT 888069-99-6P

RL: PKT (Pharmacokinetics); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of benzothiazoles, their macrogol glyceride pharmaceutical formulations, and their therapeutic use)

RN 888069-99-6 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-(4-

morpholinylmethyl)phenyl]methoxy]-4-pyrimidinyl]-, dimethanesulfonate (9CI) (CA INDEX NAME)

CM

CRN 848344-36-5 CMF C25 H23 N5 O2 S

CM 2

CRN 75-75-2 CMF C H4 O3 S

IT 848344-36-5, (1,3-Benzothiazol-2-yl)[2-[[4-[(morpholin-4-yl)methyl]benzyl]oxy]pyrimidin-4-yl]acetonitrile
RL: THU (Therapeutic use) BIOL (Biological study); USES (Uses)
(preparation of benzothiazoles, their macrogol glyceride pharmaceutical formulations, and their therapeutic use)
RN 848344-36-5 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-(4-morpholinylmethyl)phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

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L4
     ANSWER 5 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN
AN
     2005:1123763 CAPLUS
DN
     143:393032
ΤI
     Pharmaceutical composition comprising a JNK inhibitor and cyclosporin
     Rommel, Christian; Vitte, Pierre-Alain
IN
PA
     Applied Research Systems Ars Holding N. V., Neth. Antilles
     PCT Int. Appl., 102 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LA
     English
FAN.CNT 1
     PATENT NO.
                          KIND
                                 DATE
                                             APPLICATION NO.
                                                                     DATE
PΙ
     WO 2005097116
                          A1
                                 20051020
                                           WO 2005-EP51572
                                                                     20050408
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             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,
             LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA,
             NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL,
             SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA,
             ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
             RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
             MR, NE, SN, TD, TG
                                 20040408
PRAI EP 2004-101468
os
     MARPAT 143:393032
     The present invention is related to a composition comprising a c-Jun N-Terminal
     kinase (JNK) inhibitor and a cyclosporin, in particular for the treatment
     of neuronal disorders, autoimmune diseases, cancer and cardiovascular
     diseases. Neuroprotective effects of a JNK inhibitor combined with
     cyclosporin is shown in a model of global ischemia in gerbils. A JNK
     inhibitor, e.g. benzothiazole compound was admixed as a dry powder together
     with a cyclosporin and with a starch diluent in an approx. 1:1 weight ratio.
     The mixture is filled into 250 mg capsules (125 mg of active benzothiazole
     compound and 15, 25, or 50 mg of cyclosporin per capsule).
IT
     345986-40-5 345986-66-5 345986-69-8
     345986-72-3 345986-75-6 345986-78-9
     345986-81-4 345986-84-7 345986-86-9
     345986-91-6 345986-94-9 345986-96-1
     345986-98-3 345986-99-4 345987-00-0
     345987-02-2 345987-03-3 345987-04-4
     345987-06-6 345987-09-9 345987-11-3
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     848344-00-3 848344-01-4 848344-02-5
     848344-03-6 848344-04-7 .848344-06-9
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866916-18-9 866916-19-0 866916-20-3
866916-21-4 866916-22-5
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
(Biological study); USES (Uses)
   (pharmaceutical composition comprising JNK inhibitor and cyclosporin)
345986-40-5 CAPLUS
2-Benzothiazoleacetonitrile, a-(2,6-dimethoxy-4-pyrimidinyl)- (9CI)
(CA INDEX NAME)
```

RN

CN

RN 345986-66-5 CAPLUS
CN 2-Benzothiazoleacetonitrile, α-[2-(1-piperazinyl)-4-pyrimidinyl]-(90I) (CA INDEX NAME)

RN 345986-69-8 CAPLUS
CN 2-Benzothiazoleacetonitrile, \(\alpha - [2-[4-(phenylmethyl)-1-piperidinyl] - 4-pyrimidinyl] - (9CI) (CA INDEX NAME)

RN 345986-72-3 CAPLUS
CN 2-Benzothiazoleacetonitrile, α-[2-(4-methyl-1-piperazinyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 345986-75-6 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-(4-morpholinyl)-4-pyrimidinyl]-(9CI) (CA INDEX NAME)

RN 345986-78-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-(methylamino)-4-pyrimidinyl]-(9CI) (CA INDEX NAME)

RN 345986-81-4 CAPLUS

CN 2-Benzothiazoleacetonitrile, \(\alpha - [2-[4-[2-(4-morpholinyl)ethyl]-1-piperazinyl] - 4-pyrimidinyl] - (9CI) (CA INDEX NAME)

RN 345986-84-7 CAPLUS

CN 2-Benzothiazoleacetonitrile, α -[2-[4-(phenylmethoxy)-1-piperidinyl]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 345986-86-9 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-(4-hydroxy-1-piperidinyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 345986-91-6 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(dimethylamino)ethyl]amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 345986-94-9 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-(dimethylamino)-4-pyrimidinyl]-(9CI) (CA INDEX NAME)

- RN 345986-96-1 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[(2-methoxyethyl)amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 345986-98-3 CAPLUS
- CN 2-Benzothiazoleacetonitrile, \(\alpha [2-[(2-hydroxyethy1) amino] 4-pyrimidiny1] (9CI) (CA INDEX NAME)

RN 345986-99-4 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-(propylamino)-4-pyrimidinyl)-(9CI) (CA INDEX NAME)

RN 345987-00-0 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[3-(1H-imidazol-1-yl)propyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 345987-02-2 CAPLUS

CN 2-Benzothiazoleacetonitrile, α -[2-(1-pyrrolidiny1)-4-pyrimidiny1]-(9CI) (CA INDEX NAME)

RN 345987-03-3 CAPLUS

CN 2-Benzothiazoleacetonitrile, $\alpha-[2-[(2-phenylethyl)amino]-4-pyrimidinyl]-(9CI)$ (CA INDEX NAME)

RN 345987-04-4 CAPLUS

CN 2-Benzothiazoleacetonitrile, α -[2-[[2-(2-pyridinyl)ethyl]amino]-4-

pyrimidinyl] - (9CI) (CA INDEX NAME)

- RN 345987-06-6 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[(2-pyridinylmethyl)amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 345987-09-9 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[4-(1H-benzotriazol-1-yl)-1-piperidinyl]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 345987-11-3 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-(4-pyrazinyl-1-piperazinyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 345987-13-5 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[4-(2-pyrimidinyl)-1-piperazinyl]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 345987-15-7 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(3-pyridinyl)ethyl]amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 345987-17-9 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[5-bromo-2-[[2-(dimethylamino)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 345987-19-1 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-(2-methoxy-4-pyrimidinyl)- (9CI) (CA INDEX NAME)

- RN 622381-38-8 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α -[2-[[4-[4-methyl-1-piperazinyl)methyl]phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 622381-40-2 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α -[2-[[4-[[4-(phenylmethyl)-1-piperazinyl]methyl]phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 622381-42-4 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[4-[(4-ethyl-1-piperazinyl)methyl]phenyl]methoxy]- (9CI) (CA INDEX NAME)

RN 622381-43-5 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[4-[(4-(2-methoxyethyl)-1-piperazinyl]methyl]phenyl]methoxy]- (9CI) (CA INDEX NAME)

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-- OMe

RN 622381-45-7 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-(1-piperazinylmethyl)phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 622381-47-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-[(4-formyl-1-

Page 44

piperazinyl)methyl]phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 622381-49-1 CAPLUS

CN Piperazine, 1-(aminoacetyl)-4-[[4-[[4-(2(3H)-benzothiazolylidenecyanomethyl)-2-pyrimidinyl]oxy]methyl]phenyl]methyl][9CI) (CA INDEX NAME]

RN 622381-51-5 CAPLUS

CN Piperazine, 1-acetyl-4-[[4-[[4-(2-benzothiazolylcyanomethyl)-2-pyrimidinyl]oxy]methyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 622381-53-7 CAPLUS

CN 1-Piperazinecarboxamide, 4-[[4-[[4-(2(3H)-benzothiazolylidenecyanomethyl)-2-pyrimidinyl]oxy]methyl]phenyl]methyl]-N,N-dimethyl-(9CI) (CA INDEX NAME)

RN 622381-55-9 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[4-(2(3H)-benzothiazolylidenecyanomethyl)-2-pyrimidinyl]oxy]methyl]phenyl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 622381-57-1 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[4-[[4-(1,2,4-oxadiazol-3-ylmethyl)-1-piperazinyl]methyl]phenyl]methoxy]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

RN 622381-59-3 CAPLUS

CN 4-Pyrimidineacetonitrile, α -2(3H)-benzothiazolylidene-2-[[4-[[4-(2-hydroxyethyl)-1-piperazinyl]methyl]phenyl]methoxy]- (9CI) (CA INDEX NAME)

RN 622381-61-7 CAPLUS

CN l-Piperazineacetic acid, 4-[[4-[2(3H)-benzothiazolylidenecyanomethyl)-2-pyrimidinyl]oxy]methyl]phenyl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 622381-63-9 CAPLUS

CN l-Piperazineacetamide, 4-[[4-[[4-(2(3H)-benzothiazolylidenecyanomethyl)-2-pyrimidinyl]oxy]methyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 848343-80-6 CAPLUS

CN 2-Benzothiazoleacetonitrile, α -[2-[[2-(4-morpholinyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848343-82-8 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[3-(2-oxo-1-pyrrolidinyl)propyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848343-83-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, \(\alpha - [2-[methyl[3-(methylamino)propyl]amino] - 4-pyrimidinyl] - (9CI) (CA INDEX NAME)

RN 848343-86-2 CAPLUS

CN 2-Benzothiazoleacetonitrile, α -[2-[[2-(1-methyl-1H-imidazol-4-yl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848343-87-3 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(2-(1H-indol-3-y1)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848343-88-4 CAPLUS

CN 2-Benzothiazoleacetonitrile, α -[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848343-90-8 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(3-aminopropyl)amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848343-91-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(2-aminoethyl)amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848343-92-0 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[3-(dimethylamino)propyl]amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848343-93-1 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-([2-(1-piperidinyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CN & N \\ CH & N \\ N & NH-CH_2-CH_2-N \end{array}$$

RN 848343-94-2 CAPLUS

CN 2-Benzothiazoleacetonitrile, α -[2-[(phenylmethyl)amino]-4-

pyrimidinyl] - (9CI) (CA INDEX NAME)

RN 848343-95-3 CAPLUS

CN β-Alanine, N-[4-(2-benzothiazolylcyanomethyl)-2-pyrimidinyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

RN 848343-96-4 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(3-hydroxypropyl)amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848343-97-5 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(3-pyridinylmethyl)amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848343-98-6 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(4-pyridinylmethyl)amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

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- RN 848344-00-3 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(4-aminophenyl)ethyl]amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 848344-01-4 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α -[2-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 848344-02-5 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(3-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 848344-03-6 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(2-fluorophenyl)ethyl]amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ &$$

- RN 848344-04-7 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[[2-[3-(trifluoromethyl)phenyl]ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & \text{CN} & \text{N} \\ & \text{CH} & \text{N} & \text{NH-CH}_2\text{--CH}_2 \\ \end{array}$$

RN 848344-06-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-[[3-(trifluoromethyl)-2-pyridinyl]amino]ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-07-0 CAPLUS

CN 2-Benzothiazoleacetonitrile, $\alpha-[2-[(2-(3-chlorophenyl)ethyl]amino]-4-pyrimidinyl]-(9CI) (CA INDEX NAME)$

$$\begin{array}{c|c} & CN & N \\ \hline & CH & N \\ \hline & CH & NH-CH_2-CH_2 \\ \hline \end{array}$$

RN 848344-08-1 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(3,4-dichlorophenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-09-2 CAPLUS

CN 2-Benzothiazoleacetonitrile, α -[2-[[2-(4-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 848344-10-5 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(4-methylphenyl)ethyl]amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 848344-11-6 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(3-fluorophenyl)ethyl]amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 848344-12-7 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[(2-(4-phenoxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 848344-13-8 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(2-phenoxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 848344-14-9 CAPLUS
- CN 2-Benzothiazoleacetonitrile, \(\alpha [2-[[2-(4-bromophenyl)ethyl] \) amino] -4pyrimidinyl] - (9CI) (CA INDEX NAME)

RN 848344-15-0 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(4-fluorophenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\$$

RN 848344-16-1 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(2-[1,1'-biphenyl]-4-ylethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-17-2 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(4-nitrophenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-18-3 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(1H-1,2,4-triazol-1-yl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-19-4 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[3-(1H-pyrazol-1-y1)propy1]amino]-

4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-20-7 CAPLUS

CN Benzenesulfonamide, 4-[2-[[4-(2-benzothiazolylcyanomethyl)-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 848344-22-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(1H-tetrazol-5-ylmethyl)amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-23-0 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-(phenylmethoxy)-4-pyrimidinyl](9CI) (CA INDEX NAME)

RN 848344-25-2 CAPLUS

CN 2-Benzothiazoleacetonitrile, α -[2-(4-pyridinylmethoxy)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-26-3 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-(2-pyridinylmethoxy)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-28-5 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(4-methoxyphenyl)methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ &$$

- RN 848344-29-6 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α -[2-(3-pyridinylmethoxy)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-30-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, α -[2-[2-(4-methoxyphenyl)ethoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-31-0 CAPLUS

CN 2-Benzothiazoleacetonitrile, α -[2-([1,1'-biphenyl]-3-ylmethoxy)-4-

pyrimidinyl] - (9CI) (CA INDEX NAME)

RN 848344-32-1 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(3,4,5-trimethoxyphenyl)methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-33-2 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(3,4-dichlorophenyl)methoxy]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-34-3 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[3-[(dimethylamino)methyl]phenyl] methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-35-4 CAPLUS

CN 2-Benzothiazoleacetonitrile, \(\alpha = \frac{12-[(1-\text{oxido}-3-\text{pyridinyl}) \text{methoxy}]-4-\text{pyrimidinyl} - (9CI) (CA INDEX NAME)

RN 848344-36-5 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-(4-morpholinylmethyl)phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-37-6 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-(2-pyridinyl)phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-38-7 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-(1-piperidinylmethyl)phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-39-8 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-(4-methoxyphenoxy)-4-pyrimidinyl]-(9CI) (CA INDEX NAME)

- RN 848344-40-1 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-(4-butoxyphenoxy)-4-pyrimidinyl]-(9CI) (CA INDEX NAME)

- RN 848344-41-2 CAPLUS
- CN Piperazine, 1-acetyl-4-[4-[(4-(2-benzothiazolylcyanomethyl)-2-pyrimidinyl]oxy]phenyl]- (9CI) (CA INDEX NAME)

- RN 848344-70-7 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(1-methyl-1H-imidazol-5-yl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 866916-11-2 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[4-[[3-
 - [(trifluoromethyl)sulfonyl]phenyl]amino]-l-piperidinyl]-4-pyrimidinyl]-(9CI) (CA INDEX NAME)

- RN 866916-12-3 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[[3-(4-methyl-1-piperazinyl)propyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 866916-13-4 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[3-(4-morpholinyl)propyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 866916-14-5 CAPLUS

CN Carbamic acid, [4-[2-[[4-(2-benzothiazolylcyanomethyl)-2pyrimidinyl]amino]ethyl]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 866916-15-6 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(2-hydroxy-2-phenylethyl) amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 866916-17-8 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(3-pyridinyl)ethyl]amino]-5-(trifluoromethyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 866916-18-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-(3-pyridinyl)phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 866916-19-0 CAPLUS

CN 2-Benzothiazoleacetonitrile, α -[2-[3-(2-pyridinyl)propoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 866916-20-3 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-(4-methoxyphenoxy)-5-(trifluoromethyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 866916-21-4 CAPLUS

CN Benzamide, N-[2-[[4-(2-benzothiazolylcyanomethyl)-2-pyrimidinyl]amino]ethyl]-4-chloro-(9CI) (CA INDEX NAME)

RN 866916-22-5 CAPLUS

CN Glycine, N-[4-(2-benzothiazolylcyanomethyl)-2-pyrimidinyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

IT 345986-64-3

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (pharmaceutical composition comprising JNK inhibitor and cyclosporin)

RN 345986-64-3 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(1H-imidazol-4-yl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & CN & N \\ \hline & CH & N \\ N & NH-CH_2-CH_2 \\ \hline & N \\ \end{array}$$

RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/511,438

L4 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2005:1059107 CAPLUS

DN 143:472316

TI Anatomy of Fingerprint Search Calculations on Structurally Diverse Sets of Active Compounds

AU Godden, Jeffrey W.; Stahura, Florence L.; Bajorath, Juergen

CS Department of Life Science Informatics, Rheinische Friedrich-Wilhelms-Universitaet, Bonn, D-53113, Germany

SO Journal of Chemical Information and Modeling (2005), 45(6), 1812-1819 CODEN: JCISD8: ISSN: 1549-9596

PB American Chemical Society

DT Journal

LA English

AB Similarity searching using mol. fingerprints is a widely used approach for the identification of novel hits. A fingerprint search involves many pairwise comparisons of bit string representations of known active mols. with those precomputed for database compds. Bit string overlap, as evaluated by various similarity metrics, is used as a measure of mol. similarity. Results of a number of studies focusing on fingerprints suggest that it is difficult, if not impossible, to develop generally applicable search parameters and strategies, irresp. of the compound classes under investigation. Rather, more or less, each individual search problem requires an adjustment of calcn. conditions. Thus, there is a need for diagnostic tools to analyze fingerprint-based similarity searching. The authors report an anal. of fingerprint search calcns. on different sets of structurally diverse active compds. Calcns. on five biol. activity classes were carried out with two fingerprints in two compound source databases, and the results were analyzed in histograms. Tanimoto coefficient (Tc) value ranges where active compds. were detected were compared to the distribution of Tc values in the database. The anal. revealed that compound class-specific effects strongly influenced the outcome of these fingerprint calcns. Among the five diverse compound sets studied, very different search results were obtained. The anal. described here can be applied to determine Tc intervals where scaffold hopping occurs. It can also be used to benchmark fingerprint calcns. or estimate their probability of

success. IT 869584-23-6

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(fingerprint search calcns. on structurally diverse sets of active compods.)

RN 869584-23-6 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[2-(1H-imidazol-4-yl)ethyl]amino]- (9CI) (CA INDEX NAME)

RE.CNT 88 THERE ARE 88 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/511,438

- L4 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2005:485713 CAPLUS
- DN 143:172830
- TI Design and Synthesis of the First Generation of Novel Potent, Selective, and in Vivo Active (Benzothiazol-2-yl)acetonitrile Inhibitors of the c-Jun N-Terminal Kinase
- AU Gaillard, Pascale; Jeanclaude-Etter, Isabelle; Ardissone, Vittoria; Arkinstall, Steve; Cambet, Yves; Camps, Montserrat; Chabert, Christian; Church, Dennis; Cirillo, Rocco; Gretener, Denise; Halazy, Serge; Nichols, Anthony; Szyndralewiez, Cedric; Vitte, Pierre-Alain; Gotteland, Jean-Pierre
- CS Serono Pharmaceutical Research Institute, Geneva, 1228, Switz.
 SO Journal of Medicinal Chemistry (2005), 48(14), 4596-4607
- CODEN: JMCMAR; ISSN: 0022-2623 PB American Chemical Society
- DT Journal
- LA English
- OS CASREACT 143:172830
- AB Several lines of evidence support the hypothesis that c-Jun N-terminal kinase (JNKs) plays a critical role in a wide range of diseases including cell death (apoptosis)-related disorders (neurodegenerative diseases, brain, heart, and renal ischemia, epilepsy) and inflammatory disorders (multiple sclerosis, rheumatoid arthritis, inflammatory bowel diseases). Screening of an internal compound collection for inhibitors of JNK3 led to the identification of (benzothiazol-2-yl)acetonitrile derivs. as potent and selective JNK1, -2, -3 inhibitors. Starting from initial hit I [R = Cl, Rl = Br] (AS007149), the chemical and initial structure-activity relationship (SAR) of this novel and unique kinase inhibitor template were explored. Investigation of the SAR rapidly revealed that the benzothiazol-2-ylacetonitrile pyrimidine core was crucial to retain a good level of potency on rat JNK3. Therefore, I [R = Cl, Rl = H] was further optimized by exploring a number of distal combinations in place of the chlorine atom. This led to the observation that the presence of an aromatic group, two carbons away from the aminopyrimidine moiety and bearing substituents conferring hydrogen bond acceptor (HBA) properties, could improve the potency. Further improvements to the biol. and biopharmaceutical profile of the most promising compds, were performed, resulting in the discovery of I [R = 2-(3-pyridinyl)ethyl, R1 = H] (AS601245). The in vitro and in vivo anti-inflammatory potential of this new JNK inhibitor was investigated and found to demonstrate efficacy per oral route in an exptl. model of rheumatoid arthritis (RA). TΨ
- IT 861411-30-5P RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
 - (design and synthesis of novel potent, selective, and in vivo active (benzothiazol-2-yl)acetonitrile inhibitors of the c-Jun N-terminal kinase)
- RN 861411-30-5 CAPLUS
- CN 4-Pyrimidineacetonitrile, α -2(3H)-benzothiazolylidene-2-chloro-, (αZ) (9CI) (CA INDEX NAME)

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IT
     861411-31-6P 861411-33-8P 861411-35-0P
     861411-36-1P 861411-37-2P 861411-38-3P
     861411-39-4P 861411-40-7P 861411-41-8P
     861411-42-9P 861411-43-0P 861411-44-1P
     861411-45-2P 861411-46-3P 861411-47-4P
     861411-48-5P 861411-49-6P 861411-50-9P
     861411-51-0P 861411-52-1P 861411-53-2P
     861411-54-3P 861411-55-4P 861411-56-5P
     861411-57-6P 861411-58-7P 861411-59-8P
     861411-60-1P 861411-61-2P 861411-62-3P
     861411-63-4P 861411-64-5P 861411-65-6P
     861411-66-7P 861411-67-8P 861411-68-9P
     861411-69-0P 861411-70-3P 861411-71-4P
     861411-72-5P 861411-73-6P 861411-74-7P
     861411-75-8P 861411-76-9P 861411-77-0P
     861411-78-1P 861411-79-2P 861411-80-5P
     861411-81-6P 861411-82-7P 861411-83-8P
     861411-84-9P 861411-85-0P 861411-86-1P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL
     (Biological study); PREP (Preparation)
        (design and synthesis of novel potent, selective, and in vivo active
        (benzothiazol-2-yl)acetonitrile inhibitors of the c-Jun N-terminal
        kinase)
RN
     861411-31-6 CAPLUS
CN
     4-Pyrimidineacetonitrile, \alpha-2(3H)-benzothiazolylidene-2-chloro-6-
     methyl-, (aZ)- (9CI) (CA INDEX NAME)
```

Double bond geometry as shown.

RN 861411-33-8 CAPLUS CN 4-Pyrimidineacetonitrile, 2-chloro-α-(5-(trifluoromethyl)-2(3H)-benzothiazolylidene]-, (αZ)- (9CI) (CA INDEX NAME)

RN 861411-35-0 CAPLUS

CN 4-Pyrimidineacetonitrile, 2-chloro-α-(3-methyl-2(3H)-benzothiazolylidene)-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-36-1 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-, (αZ)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-37-2 CAPLUS

CN 4-Pyrimidineacetonitrile, 2-amino- α -2(3H)-benzothiazolylidene-, (α Z)- (9CI) (CA INDEX NAME)

RN 861411-38-3 CAPLUS
CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-hydrazino-,
(αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-39-4 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-(methylamino)-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-40-7 CAPLUS

CN 4-Pyrimidineacetonitrile, α -2(3H)-benzothiazolylidene-2-(dimethylamino)-, (α Z)- (9CI) (CA INDEX NAME)

RN 861411-41-8 CAPLUS CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-(1-piperazinyl)-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-42-9 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-(4-methyl-1-piperazinyl)-, (α2)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-43-0 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-(4-morpholinyl)-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-44-1 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-(1-pyrrolidinyl)-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-45-2 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-(4-hydroxy-1-piperidinyl)-, (αZ)- (9CI) (CA INDEX NAME)

RN 861411-46-3 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[2-(dimethylamino)ethyl]amino]-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-47-4 CAPLUS

CN 4-Pyrimidineacetonitrile, 2-[(2-aminoethyl)amino]- α -2(3H)-benzothiazolylidene-, (α Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-48-5 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[(2-methoxyethyl)amino]-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-49-6 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[(2-hydroxyethyl)amino]-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-50-9 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-(propylamino)-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-51-0 CAPLUS

CN 4-Pyrimidineacetonitrile, α -2(3H)-benzothiazolylidene-2-[[2-(1-piperidinyl)ethyl]amino]-, (αZ) - (9CI) (CA INDEX NAME)

RN 861411-52-1 CAPLUS
CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[2-(4-morpholinyl)ethyl]amino]-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-53-2 CAPLUS

CN

4-Pyrimidineacetonitrile, α -2(3H)-benzothiazolylidene-2-[[3-(dimethylamino)propyl]amino]-, (αZ) - (9CI) (CA INDEX NAME)

RN 861411-54-3 CAPLUS

CN 4-Pyrimidineacetonitrile, 2-[(3-aminopropyl)amino]- α -2(3H)-benzothiazolylidene-, (α 2)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-55-4 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[(3-hydroxypropyl)amino]-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-56-5 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[3-(4-morpholinyl)propyl]amino]-, (α2)- (9CI) (CA INDEX NAME)

RN 861411-57-6 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[3-(4-methyl-1-piperazinyl)propyl]amino]-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-58-7 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[3-(2-oxo-1-pyrrolidinyl)propyl]amino]-, (αZ)- (9CI) (CA INDEX NAME)

RN 861411-59-8 CAPLUS
CN 4-Pyrimidineacetonitrile, α-2(3)

4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[methyl[3-(methylamino)propyl]amino]-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-60-1 CAPLUS

CN 4-Pyrimidineacetonitrile, \alpha-2(3H)-benzothiazolylidene-2[(phenylmethyl)amino]-, (\alpha Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-61-2 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[(2-pyridinylmethyl)amino]-, (αZ)- (9CI) (CA INDEX NAME)

RN 861411-62-3 CAPLUS
CN 4-Pyrimidineacetonitrile, α -2(3H)-benzothiazolylidene-2-[(3-pyridinylmethyl)amino]-, $(\alpha$ Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-63-4 CAPLUS

CN 4-Pyrimidineacetonitrile, α -2(3H)-benzothiazolylidene-2-[(4-pyridinylmethyl)amino]-, (α Z)- (9CI) (CA INDEX NAME)

RN 861411-64-5 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[(2H-tetrazol-2-ylmethyl)amino]-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-65-6 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[(2-phenylethyl)amino]-, (αZ)- (9CI) (CA INDEX NAME)

- RN 861411-66-7 CAPLUS
- CN 4-Pyrimidineacetonitrile, \(\alpha 2(3\text{H}) \text{benzothiazolylidene-2-[[2-(2-fluorophenyl)ethyl]amino]-, (\alpha Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

- RN 861411-67-8 CAPLUS
- CN 4-Pyrimidineacetonitrile, $\alpha-2(3H)$ -benzothiazolylidene-2-[[2-(3-fluorophenyl)ethyl]amino]-, (αZ) (9CI) (CA INDEX NAME)

RN 861411-68-9 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[2-(4-fluorophenyl)ethyl]amino]-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-69-0 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[2-[2-(3-chlorophenyl)ethyl]hydrazino]-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-70-3 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[2-[2-(3,4-dichlorophenyl)ethyl]hydrazino]-, (αZ)- (9CI) (CA INDEX NAME)

RN 861411-71-4 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[2-[2-(4-bromophenyl)ethyl]hydrazino]-, (αΣ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-72-5 CAPLUS

CN 4-Pyrimidineacetonitrile, α -2(3H)-benzothiazolylidene-2-[[2-(4-methylphenyl)ethyl]amino]-, $(\alpha 2)$ - (9CI) (CA INDEX NAME)

RN 861411-73-6 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[2-(4-hydroxyphenyl)ethyl]amino]-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-74-7 CAPLUS

CN 4-Pyrimidineacetonitrile, α -2(3H)-benzothiazolylidene-2-[[2-(4-methoxyphenyl)ethyl]amino]-, (αZ) - (9CI) (CA INDEX NAME)

RN 861411-75-8 CAPLUS

CN 4-Pyrimidineacetonitrile, 2-[[2-(4-aminophenyl)ethyl]amino]-α-2(3H)-benzothiazolylidene-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-76-9 CAPLUS

CN Benzenesulfonamide, 4-[2-[[4-[(Z)-2(3H)-benzothiazolylidenecyanomethyl]-2pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 861411-77-0 CAPLUS
CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[2-(4-nitrophenyl)ethyl]amino]-, (α2)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-78-1 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[2-(1H-indol-3-yl)ethyl]amino]-, (αZ)- (9CI) (CA INDEX NAME)

RN 861411-79-2 CAPLUS
CN 4-Pyrimidineacetonitrile, \(\alpha - 2 \) (3H) -benzothiazolylidene-2-[[2-(1H-imidzo1-4-yl)ethyl]amino]-, \(\alpha Z) - \) (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-80-5 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[2-(1-methyl-1H-imidazol-4-yl)ethyl]amino]-, (αZ)- (9CI) (CA INDEX NAME)

RN 861411-81-6 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[(2-(1-methyl-1H-imidazol-2-yl)ethyl]amino]-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-82-7 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[2-(2-pyridinyl)ethyl]amino]-, (αZ)- (9CI) (CA INDEX NAME)

RN 861411-83-8 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[2-(3-pyridinyl)ethyl]amino]-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 861411-84-9 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2 (3H)-benzothiazolylidene-2-[[2-(1H-1,2,4-triazol-1-yl)ethyl]amino]-, (αZ)- (9CI) (CA INDEX NAME)

RN 861411-85-0 CAPLUS CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[3-(1H-imidazol-1-yl)propyl]amino]-, (α2)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN . 861411-86-1 CAPLUS

CN 4-Pyrimidineacetonitrile, α -2(3H)-benzothiazolylidene-2-[[3-(1H-pyrazol-1-yl)propyl]amino]-, (α Z)- (9CI) (CA INDEX NAME)

RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ANSWER 8 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN
L4
AN
     2005:259876 CAPLUS
DN
     142:341891
ТT
     Benzothiazole derivatives for the treatment of diabetes
     Gaillard, Pascale; Gotteland, Jean-Pierre; Vitte, Pierre-Alain
TN
PA
     Applied Research Systems ARS Holding N.V., Neth. Antilles
SO
     PCT Int. Appl., 46 pp.
     CODEN: PTXXD2
DT
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LA
     English
FAN.CNT 1
     PATENT NO.
                         KIND
                                DATE
                                            APPLICATION NO.
                                                                     DATE
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PT
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                                20060407
     NO 2006001600
                                            NO 2006-1600
                                                                     20060407
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PRAI EP 2003-102740
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                          А
     WO 2004-EP52090
                          W
                                20040908
OS
     MARPAT 142:341891
AB
     The present invention is related to the use of benzothiazole derivs. for
     the manufacture of a medicament for the treatment of metabolic disorders
     mediated by insulin resistance or hyperglycemia, comprising diabetes type
     II, inadequate glucose tolerance, insulin resistance, obesity, polycystic
     ovary syndrome (PCOS) Formula I. G is an unsubstituted or substituted
     pyrimidinyl group. L is an unsubstituted or substituted C1-C6-alkoxy, or
     an amino group, or an unsubstituted or a substituted 3-8 membered
     heterocycloalkyl, containing at least one heteroatom selected from N, O, S
     (e.g. a piperazine, a piperidine, a morpholine, a pyrrolidine). R1 is
     selected from the group comprising or consisting of hydrogen, sulfonyl,
    amino, unsubstituted or substituted C1-C6-alkyl, unsubstituted or
     substituted C2-C6-alkenyl, unsubstituted or substituted C2-C6-alkynyl or
     C1-C6-alkoxy, unsubstituted or substituted aryl, halogen, cyano or
     hydroxy. Efficacy of benzothiazole derivs. in exptl. model of type II
     diabetes was studied. Oral formulations of benzothiazole compound of
     formula I is described.
     345986-40-5 345986-64-3 345986-66-5
IT
     345986-69-8 345986-72-3 345986-75-6
     345986-78-9 345986-81-4 345986-84-7
     345986-86-9 345986-91-6 345986-94-9
     345986-96-1 345986-98-3 345986-99-4
     345987-00-0 345987-02-2 345987-03-3
     345987-04-4 345987-06-6 345987-09-9
     345987-11-3 345987-13-5 345987-15-7
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848344-57-0 848344-58-1 848344-70-7
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
(Biological study); USES (Uses)
   (benzothiazole derivs. for treatment of diabetes)
345986-40-5 CAPLUS
2-Benzothiazoleacetonitrile, α-(2,6-dimethoxy-4-pyrimidinyl)- (9CI)
(CA INDEX NAME)
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RN.

CN

RN 345986-64-3 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(1H-imidazol-4-yl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CN & N & H \\ \hline CH & N & NH-CH_2-CH_2 \\ \hline \end{array}$$

RN 345986-66-5 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-(1-piperazinyl)-4-pyrimidinyl]-

(9CI) (CA INDEX NAME)

RN 345986-69-8 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[4-(phenylmethyl)-1-piperidinyl]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 345986-72-3 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-(4-methyl-1-piperazinyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 345986-75-6 CAPLUS

CN 2-Benzothiazoleacetonitrile, α -[2-(4-morpholinyl)-4-pyrimidinyl]-(9CI) (CA INDEX NAME)

RN 345986-78-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, α -[2-(methylamino)-4-pyrimidinyl]-(9CI) (CA INDEX NAME)

- RN 345986-81-4 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[4-[2-(4-morpholinyl)ethyl]-1-piperazinyl]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 345986-84-7 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[4-(phenylmethoxy)-1-piperidinyl]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 345986-86-9 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-(4-hydroxy-1-piperidinyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 345986-91-6 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(dimethylamino)ethyl]amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 345986-94-9 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-(dimethylamino)-4-pyrimidinyl]-(9CI) (CA INDEX NAME)

RN 345986-96-1 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(2-methoxyethyl)amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 345986-98-3 CAPLUS

CN 2-Benzothiazoleacetonitrile, \(\alpha - [2-[(2-hydroxyethyl)amino] - 4-pyrimidinyl] - (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{CN} & \text{N} \\ & \text{CH} & \text{NH-CH}_2\text{-CH}_2\text{-OH} \\ \end{array}$$

RN 345986-99-4 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-(propylamino)-4-pyrimidinyl]-(9CI) (CA INDEX NAME)

RN 345987-00-0 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[3-(1H-imidazol-1-yl)propyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 345987-02-2 CAPLUS

CN 2-Benzothiazoleacetonitrile, α -[2-(1-pyrrolidinyl)-4-pyrimidinyl]-

(9CI) (CA INDEX NAME)

RN 345987-03-3 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(2-phenylethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 345987-04-4 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(2-pyridinyl)ethyl]amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 345987-06-6 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(2-pyridinylmethyl)amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 345987-09-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[4-(1H-benzotriazol-1-yl)-1-piperidinyl]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 345987-11-3 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-(4-pyrazinyl-1-piperazinyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 345987-13-5 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[4-(2-pyrimidinyl)-1-piperazinyl]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 345987-15-7 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(3-pyridinyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 345987-17-9 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[5-bromo-2-[[2-(dimethylamino)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 848343-80-6 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(4-morpholinyl)ethyl]amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848343-81-7 CAPLUS
CN 2-Benzothiazoleacetonitrile, \(\alpha\text{-[2-[4-[[3-[\text{[trifluoromethyl]} sulfonyl]]phenyl]methyl]-1-piperidinyl]-4-pyrimidinyl]-\((9CI\) (CA INDEX NAME)

RN 848343-82-8 CAPLUS

CN 2-Benzothiazoleacetonitrile, \(\alpha - [2-[[3-(2-\infty - 1-\infty - 1-\

RN 848343-83-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[methyl[3-(methylamino)propyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848343-84-0 CAPLUS

CN 2-Benzothiazoleacetonitrile, α -[2-[[3-[(4-methyl-1-piperazinyl)amino]propyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848343-85-1 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[3-(4-morpholinylamino)propyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848343-86-2 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(1-methyl-1H-imidazol-4-yl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} S & CH & N \\ \hline & CH & N \\ \hline & NH-CH_2-CH_2 \\ \hline & N \\ \end{array}$$

RN 848343-87-3 CAPLUS

CN 2-Benzothiazoleacetonitrile, α -[2-[[2-(1H-indol-3-yl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848343-88-4 CAPLUS

CN 2-Benzothiazoleacetonitrile, \(\alpha - [2-[[2-(4-hydroxyphenyl)ethyl]amino] - 4-pyrimidinyl] - (9CI) (CA INDEX NAME)

RN 848343-89-5 CAPLUS

CN Carbamic acid, [4-(2-benzothiazolylcyanomethyl)-2-pyrimidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 848343-90-8 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(3-aminopropyl)amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848343-91-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(2-aminoethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848343-92-0 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[3-(dimethylamino)propyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848343-93-1 CAPLUS

CN 2-Benzothiazoleacetonitrile, \alpha-[2-[[2-(1-piperidinyl)ethyl]amino]-4-

pyrimidinyl] - (9CI) (CA INDEX NAME)

- RN 848343-94-2 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[(phenylmethyl)amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 848343-95-3 CAPLUS
- CN β-Alanine, N-[4-(2-benzothiazolylcyanomethyl)-2-pyrimidinyl]-, l-methylethyl ester (9CI) (CA INDEX NAME)

- RN 848343-96-4 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[(3-hydroxypropyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 848343-97-5 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[(3-pyridinylmethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 848343-98-6 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[(4-pyridinylmethyl)amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 848343-99-7 CAPLUS
- CN Carbamic acid, (1,1-dimethylethyl)-, 4-[2-[[4-(2-benzothiazolylcyanomethyl)-2-pyrimidinyl]amino]ethyl]phenyl ester (9CI) (CA INDEX NAME)

- RN 848344-00-3 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[(2-(4-aminophenyl)ethyl]amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 848344-01-4 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 848344-02-5 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α -[2-[[2-(3-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-03-6 CAPLUS

CN 2-Benzothiazoleacetonitrile, \(\alpha - [2-[[2-(2-fluorophenyl)ethyl]amino] - 4-pyrimidinyl] - (9CI) (CA INDEX NAME)

RN 848344-04-7 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-[3-(trifluoromethyl)phenyl]ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-05-8 CAPLUS

CN 2-Benzothiazoleacetonitrile, α -[2-[(2-(2-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-06-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[3-(trifluoromethyl)-2-pyridinyl]amino]ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-07-0 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(3-chlorophenyl)ethyl]amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-08-1 CAPLUS

CN 2-Benzothiazoleacetonitrile, a-[2-[[2-(3,4-dichlorophenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-09-2 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(4-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-10-5 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(4-methylphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-11-6 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(3-fluorophenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-12-7 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(2-(4-phenoxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-13-8 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(2-phenoxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-14-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(2-(4-bromophenyl)ethyl]amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-15-0 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(4-fluorophenyl)ethyl]amino]-4pyrimidinyl]- (9CI) (ČA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & &$$

RN 848344-16-1 CAPLUS

CN 2-Benzothiazoleacetonitrile, α -[2-[(2-[1,1'-biphenyl]-4-

10/511.438

vlethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 848344-17-2 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(4-nitrophenyl)ethyl]amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 848344-18-3 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(1H-1,2,4-triazol-1-yl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 848344-19-4 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[[3-(1H-pyrazol-1-yl)propyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 848344-20-7 CAPLUS
- CN Benzenesulfonamide, 4-[2-[[4-(2-benzothiazolylcyanomethyl)-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 848344-21-8 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(2-(2-pyridinyl)ethyl]amino]-4pyrimidinyl]-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 848344-22-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(1H-tetrazol-5-ylmethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-23-0 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-(phenylmethoxy)-4-pyrimidinyl]-(9CI) (CA INDEX NAME)

RN 848344-24-1 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[3-(4-pyridinyl)phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 848344-25-2 CAPLUS
- CN 2-Benzothiazoleacetonitrile, \(\alpha [2-(4-pyridinylmethoxy)-4-pyrimidinyl] (9CI) (CA INDEX NAME)

- RN 848344-26-3 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-(2-pyridinylmethoxy)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 848344-27-4 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[3-(3-pyridinyl)propoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 848344-28-5 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[(4-methoxyphenyl)methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

- RN 848344-29-6 CAPLUS
- CN 2-Benzothiazoleacetonitrile, \(\alpha [2-(3-pyridinylmethoxy) 4-pyrimidinyl] (9CI) (CA INDEX NAME)

RN 848344-30-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, \(\alpha - \left[2-\left[2-\left(4-\text{methoxyphenyl}\right)] + \right] - \(\text{pyrimidinyl} \right] - \(\left(\text{CA INDEX NAME} \right) \)

RN 848344-31-0 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-([1,1'-biphenyl]-3-ylmethoxy)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-32-1 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(3,4,5-trimethoxyphenyl)methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-33-2 CAPLUS

CN 2-Benzothiazoleacetonitrile, α -[2-[(3,4-dichlorophenyl)methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-34-3. CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[3-[(dimethylamino)methyl]phenyl] methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-35-4 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(1-oxido-3-pyridinyl)methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-36-5 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-(4-morpholinylmethyl)phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-37-6 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-(2-pyridinyl)phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-38-7 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-(1-piperidinylmethyl)phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-39-8 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-(4-methoxyphenoxy)-4-pyrimidinyl](9CI) (CA INDEX NAME)

RN 848344-40-1 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-(4-butoxyphenoxy)-4-pyrimidinyl]-(9CI) (CA INDEX NAME)

RN 848344-41-2 CAPLUS

CN Piperazine, 1-acetyl-4-[4-[2-benzothiazolylcyanomethyl)-2pyrimidinyl]oxy]phenyl]- (9CI) (CA INDEX NAME)

RN 848344-42-3 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-(4-methoxyphenoxy)-4-pyrimidinyl]-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 848344-43-4 CAPLUS

CN Benzamide, 4-chloro-N-[4-[cyano[6-(trifluoromethyl)-2-benzothiazolyl]methyl]-2-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-44-5 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-(2-methoxy-4-pyrimidinyl)-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 848344-45-6 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-[(4-methyl-1piperazinyl]methyl]phenyl]methoxy]-4-pyrimidinyl]-6-(trifluoromethyl)-(9CI) (CA INDEX NAME)

RN 848344-46-7 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-[[4-(phenylmethyl)-1-piperazinyl]methyl]phenyl]methoxy]-4-pyrimidinyl]-6-(trifluoromethyl)-(9CI) (CA INDEX NAME)

F3C
$$\stackrel{CN}{\longrightarrow}$$
 $\stackrel{N}{\longrightarrow}$ $\stackrel{CH_2}{\longrightarrow}$ $\stackrel{CH_2}{\longrightarrow}$

PAGE 1-B

--- Ph

RN 848344-47-8 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-(1-piperazinylmethyl) phenyl]methoxy]-4-pyrimidinyl]-6-(trifluoromethyl)-(9CI) (CA INDEX NAME)

RN 848344-48-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-[(4-formyl-1piperazinyl)methyl]phenyl]methoxy]-4-pyrimidinyl]-6-(trifluoromethyl)-(9C1) (CA INDEX NAME)

RN 848344-49-0 CAPLUS

CN Piperazine, 1-acetyl-4-[[4-[[4-[cyano[6-(trifluoromethyl)-2benzothiazolyl]methyl]-2-pyrimidinyl]oxy]methyl]phenyl]methyl]- [9CI) (CA INDEX NAME)

- RN 848344-50-3 CAPLUS
- CN 4-Pyrimidineacetonitrile, 2-[[4-[[4-(1,2,4-oxadiazol-3-ylmethyl]-1-piperazinyl]methyl]phenyl]methoxy]-a-[6-(trifluoromethyl)-2(3H)-benzothiazolylidene]- (9CI) (CA INDEX NAME)
 - PAGE 1-A

PAGE 1-B

- RN 848344-51-4 CAPLUS
- CN 1-Piperazinecarboxylic acid, 4-[[4-[[4-[cyano[6-(trifluoromethyl)-2(3H)-benzothiazolylidene]methyl]-2-pyrimidinyl]oxy]methyl]phenyl]methyl]-, methyl ester [9C1] (CA INDEX NAME)

$$F_3C \longrightarrow N \\ NH \longrightarrow N \\ O-CH_2 \longrightarrow CH_2 - N$$

- RN 848344-52-5 CAPLUS
- CN 1-Piperazineacetamide, 4-[[4-[[4-[cyano[6-(trifluoromethyl)-2(3H)-benzothiazolylidene]methyl]-2-pyrimidinyl]oxy]methyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

RN 848344-53-6 CAPLUS

CN Piperazine, 1-(aminoacetyl)-4-[[4-[[[4-[cyano[6-(trifluoromethyl)-2(3H)-benzothiazolylidene]methyl]-2-pyrimidinyl]oxy]methyl]phenyl]methyl]- (9CI) (CA INDEX NNBL)

F3C NH O-CH2 CH2-N

PAGE 1-B

- cн₂- мн₂

RN 848344-54-7 CAPLUS

CN 1-Piperazineacetic acid, 4-[[4-[[4-[[4-[cyano[6-(trifluoromethyl)-2(3H)-benzothiazolylidene]methyl]-2-pyrimidinyl]oxy]methyl]phenyl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

- RN 848344-55-8 CAPLUS
- CN 4-Pyrimidineacetonitrile, 2-[[4-[[4-(2-methoxyethyl)-1-piperazinyl]methyl]phenyl]methoxy]-α-[6-(trifluoromethyl)-2(3H)-benzothiazolylidene]-(9CI) (CA INDEX NAME)

F3C CH2 CH2 CH2 CH2 CH2 CH2

PAGE 1-B

- -- CH₂-- ОМе
- RN 848344-56-9 CAPLUS
- CN 1-Piperazinecarboxamide, 4-[[4-[[4-[cyano[6-(trifluoromethyl)-2(3H)-benzothiazolylidene]methyl]-2-pyrimidinyl]oxy]methyl]phenyl]methyl]-N,N-dimethyl- (9Cl) (CA INDEX NAME)

- RN 848344-57-0 CAPLUS
- CN 4-Pyrimidineacetonitrile, 2-[[4-[(4-ethyl-1-piperazinyl)methyl]phenyl]meth xy]- α -[6-(trifluoromethyl)-2(3H)-benzothiazolylidene]- (9CI) (CA INDEX NAME)

- RN 848344-58-1 CAPLUS
- CN 4-Pyrimidineacetonitrile, 2-[[4-[[4-(2-hydroxyethyl)-1-piperazinyl]methyl]phenyl]methoxy]-a-[6-(trifluoromethyl)-2(3H)-benzothiazolylidene]- (9GI) (CA INDEX NAME)

PAGE 1-B

- сн2 он
- RN 848344-70-7 CAPLUS
- CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(1-methyl-1H-imidazol-5-yl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/511.438

L4 ANSWER 9 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2005:233187 CAPLUS

DN 142:259314

TI. Control of death receptor and mitochondrial-dependent apoptosis by c-Jun N-terminal kinase in hippocampal CAI neurones following global transient ischemia

AU Carboni, Sonia; Antonsson, Bruno; Gaillard, Pascale; Gotteland, Jean-Pierre; Gillon, Jean-Yves; Vitte, Pierre-Alain

CS Department of Pharmacology, Serono Pharmaceutical Research Institute, Geneva, 1228, Switz.

SO Journal of Neurochemistry (2005), 92(5), 1054-1060 CODEN: JONRAS: ISSN: 0022-3042

PB Blackwell Publishing Ltd.

DT Journal

LA English

AB C-Jun N-terminal kinase (JNK), a member of the mitogen-activated protein kinase family, is activated in response to a number of extracellular stimuli, including inflammatory cytokines, UV irradiation and ischemia. A large body of evidence supports a role for JNK signaling in stress-induced apoptosis. It has been hypothesized that JNK may contribute to the apoptotic response by regulating the intrinsic cell death pathway involving the mitochondria. Here, we examined the role of the JNK signaling pathway in hippocampal CA1 apoptotic neurons following transient ischemia in gerbils. We showed early activation of death receptor-dependent apoptosis (caspase-8 activation 2 days after ischemia) and a biphasic activation of caspase-3 and caspase-9 after ischemia. Activation of the mitochondrial pathway, as measured by cytochrome c release, appeared as a late event (5-7 days after ischemia). AS601245, a novel JNK inhibitor, antagonized activation of both pathways and significantly protected CA1 neurons from cell death. Our results suggest a key role of JNK in the control of death receptor and mitochondrial-dependent apoptosis after transient ischemia.

IT 345987-15-7, As601245
RL: BUU (Biological use, unclassified); PAC (Pharmacological activity);
THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(A5601245, JNK inhibitor, antagonized activation of apoptotic and significantly protected CAI neurons from cell death.)

RN 345987-15-7 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(3-pyridinyl)ethyl]amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2005:146539 CAPLUS
- DN 142:328799
- TI Targeting the JNK signaling pathway for stroke and Parkinson's diseases therapy
- AU Kuan, Chia-Yi; Burke, Robert E.
- CS Division of Developmental Biology, Cincinnati Children's Hospital Research Foundation, Cincinnati, OH, 45229, USA
- SO Current Drug Targets: CNS & Neurological Disorders (2005), 4(1), 63-67 CODEN: CDTCCC; ISSN: 1568-007X
- PB Bentham Science Publishers Ltd.
- DT Journal; General Review
- LA English
- AB A review. The c-Jun NH2-terminal Kinase (JNK) signaling pathway is frequently induced by cellular stress and correlated with neuronal death. This unique property makes JNK signaling a promising target for developing pharmacol. intervention. Among several neurol. disorders, JNK signaling is particularly implicated in ischemic stroke and Parkinson's disease. The inhibitors of the JNK signaling pathway include upstream kinase inhibitors (for example, CEP-1347), small chemical inhibitors of JNK (SP600125 and AS601245), and peptide inhibitors of the interaction between JNK and its substrates (D-JNKI and I-JTP). The mechanisms by which JNK signaling induces apoptosis and evidence of cytoprotective effects of these JNK inhibitors are summarized in the present review.
- IT 345987-15-7, AS601245 RI: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (targeting the JNK signaling pathway for stroke and Parkinson's diseases therapy)
- . RN 345987-15-7 CAPLUS
 - CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(3-pyridinyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RE.CNT 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

T.4 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN

ΔN 2004:638580 CAPLUS

DN 141:325444

Inhibition of c-jun N-terminal kinase decreases cardiomyocyte apoptosis ΤТ and infarct size after myocardial ischemia and reperfusion in anaesthetized rats

Ferrandi, Chiara; Ballerio, Rossana; Gaillard, Pascale; Giachetti, AII Claudio; Carboni, Sonia; Vitte, Pierre-Alain; Gotteland, Jean-Pierre; Cirillo, Rocco

Instituto di Ricerche Biomediche "A. Marxer", LCG-RBM/Serono Discovery, CS Colleretto Giacosa, I-10010, Italy

British Journal of Pharmacology (2004), 142(6), 953-960 SO

CODEN: BJPCBM; ISSN: 0007-1188

Nature Publishing Group PB

DT Journal

LΑ English

AB 1 Myocardial ischemia/reperfusion is associated with inflammation, apoptosis and necrosis. During this process, c-jun N-terminal kinase is activated in cardiac myocytes resulting in apoptosis. 2 This study investigates the effects of AS601245, a nonpeptide ATP competitive JNK inhibitor, on infarct size caused by myocardial ischemia/reperfusion in anesthetized rats. The left descending coronary artery of anesthetized rats was occluded for 30 min and then reperfused for 3 h. AS601245 was administered 5 min before the end of the ischemia period as an i.v. bolus (1.5, 4.5 or 15 mg kg-1 i.v.) followed by continuous i.v. infusion (18, 55 and 183 µg kg-1 min-1, resp.) during reperfusion. Controls received saline only. 3-Aminobenzamide, a poly(ADP-ribose) polymerase inhibitor, was used as reference compound at 10 mg kg-1 i.v. bolus plus 0.17 mg kg-1 min-1 continuous infusion. 3 AS601245 significantly reduced infarct size at 4.5 mg kg-1 (-44%) and 15 mg kg-1 i.v. (-40.3%) similarly to 3-aminobenzamide (-44.2%). This protective effect was obtained without affecting hemodynamics or reducing ST-segment displacement. 4 The beneficial effects on infarct size correlated well with the reduction of c-jun phosphorvlation (-85%; vs. control) and of TUNEL-pos. cells (-82.1%) in post-ischemic cardiomyocytes. No change in the phosphorylation state of p38 MAPK and ERK in post-ischemic heart was observed in the presence of AS601245 in comparison to the vehicle-treated group. 5 These results demonstrate that blocking the JNK pathway may represent a novel therapeutic approach for treating myocardial ischemia/reperfusion-induced cardiomyocyte death.

IT 345987-15-7, AS 601245

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(inhibition of c-jun N-terminal kinase with AS601245 decreases cardiomyocyte apoptosis and infarct size after myocardial ischemia and reperfusion in anesthetized rats)

RN 345987-15-7 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(3-pyridinyl)ethyl]amino]-4pyrimidinyl] - (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{CN} \\ \text{CH} \\ \text{N} \end{array} \text{NH-CH}_2\text{-CH}_2 \\ \text{NN} \\ \text{NN} \\ \text{NH-CH}_2\text{-CH}_2 \\ \text{NN} \\$$

RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

T.4 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2004:547002 CAPLUS

DN 141:218787

TI AS601245 (1.3-benzothiazol-2-vl (2-{[2-(3-pyridinyl) ethyl] amino}-4 pyrimidinyl) acetonitrile): A c-Jun NH2-terminal protein kinase inhibitor with neuroprotective properties

Carboni, Sonia; Hiver, Agnes; Szyndralewiez, Cedric; Gaillard, Pascale; Gotteland, Jean-Pierre: Vitte, Pierre-Alain

CS Department of Pharmacology, Serono Pharmaceutical Research Institute, Geneva, Switz.

so Journal of Pharmacology and Experimental Therapeutics (2004), 310(1),

CODEN: JPETAB; ISSN: 0022-3565

PB American Society for Pharmacology and Experimental Therapeutics

DT Journal

LA English

AB Recent evidence suggests that activation of the c-Jun NH2-terminal protein kinase (JNK) signal transduction pathway may play a role in ischemia-induced cell death. Thus, preventing the activation of JNK, or c-Jun phosphorylation could be neuroprotective. In the current study, we report that a small mol., AS601245 (1,3-benzothiazol-2-yl-(2-([2-(3pyridinyl)ethyl]amino}-4-pyrimidinyl) acetonitrile), which has been shown to inhibit the JNK signaling pathway, promotes cell survival after cerebral ischemia. In vivo, AS601245 (40, 60, and 80 mg/kg) administered i.p. provided significant protection against the delayed loss of hippocampal CAl neurons in a gerbil model of transient global ischemia. This effect is mediated by JNK inhibition and therefore by c-Jun expression and phosphorylation. A significant neuroprotective effect of AS601245 administered either by i.p. injection (6, 18, and 60 mg/kg) or as i.v. bolus (1 mg/kg) followed by an i.v. infusion (0.6 mg/kg/h) was also observed in rats after focal cerebral ischemia. These data suggest that the use of JNK inhibitors such as AS601245 may be a relevant strategy in the therapy of ischemic insults.

345987-15-7, AS 601245 TT RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(JNK inhibitor AS601245 with neuroprotective properties) ВN

345987-15-7 CAPLUS

CN 2-Benzothiazoleacetonitrile, \(\alpha - [2-[[2-(3-pvridinvl)ethvl]amino] - 4pyrimidinyl] - (9CI) (CA INDEX NAME)

THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L4
     ANSWER 13 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN
AN
     2003:875284 CAPLUS
DN
     139:364962
тΤ
     Preparation of piperazine benzothiazoles as agents for the treatment of
     cerebral ischemic disorders or CNS disorders
TN
     Gaillard, Pascale; Gotteland, Jean-pierre; Vitte, Pierre-alain
PΔ
     Applied Research Systems Ars Holding N.V., Neth. Antilles
     PCT Int. Appl., 46 pp.
SO
     CODEN: PIXXD2
DT
     Patent
     English
T.A
FAN.CNT 1
     PATENT NO.
                          KIND
                                  DATE
                                              APPLICATION NO.
                                                                       DATE
     WO 2003091249
                                  20031106
                                              WO 2003-EP4323
                                                                       20030425
PT
                           A1
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             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
             PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT,
             TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     CA 2481763
                                              CA 2003-2481763
                           AA
                                  20031106
                                                                       20030425
                                              AU 2003-233067
     AU 2003233067
                           A1
                                                                       20030425
     EP 1501828
                                  20050202
                                              EP 2003-727365
                           A1
                                                                       20030425
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     CN 1662528
                                  20050831
                                              CN 2003-814493
                           Α
                                                                       20030425
     JP 2006504631
                           Т2
                                  20060209
                                              JP 2003-587807
                                                                       20030425
     ZA 2004008023
                                              ZA 2004-8023
                           А
                                  20051005
                                                                       20041005
     US 2005261304
                           A1
                                  20051124
                                              US 2005-511438
                                                                       20050610
PRAI EP 2002-100417
                           А
                                  20020425
     WO 2003-EP4323
                                  20030425
                           W
     MARPAT 139:364962
os
     The title compds. [I; R = H, alkyl, heteroaryl, etc.; R1 = H, halo, CN,
AB
     etc.; n = 0-31 and their salts that are inhibitors of JNK kinases, in
     particular of JNK2 and JNK3, and may therefore be used in the treatment
     and/or prophylaxis of cerebral ischemic disorders or CNS disorders, were
     prepared and formulated. Thus, treating alc. II with NaH in DMA followed by
     addition of the benzothiazole III (prepns. of reactants given) afforded I [R
     = Me; R1 = H; n = 1]. The tested compds. I display IC50 of < 10 μM
     with regard to JNK3.
TT
     622381-38-8P 622381-39-9P 622381-40-2P
     622381-41-3P 622381-42-4P 622381-43-5P
     622381-44-6P 622381-45-7P 622381-46-8P
     622381-47-9P 622381-48-0P 622381-49-1P
     622381-50-4P 622381-51-5P 622381-52-6P
     622381-53-7P 622381-54-8P 622381-55-9P
     622381-56-0P 622381-57-1P 622381-58-2P
     622381-59-3P 622381-60-6P 622381-61-7P
     622381-62-8P 622381-63-9P 622381-64-0P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (preparation of piperazine benzothiazoles as inhibitors of JNK kinases)
```

RN 622381-38-8 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-[(4-methyl-1-piperazinyl)methyl]phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 622381-39-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, α -[2-[[4-[(4-methyl-1-piperaziny])methyl]phenyl]methoxy]-4-pyrimidinyl]-, trimethanesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 622381-38-8

CMF C26 H26 N6 O S

CM 2

CRN 75-75-2

CMF C H4 03 S

RN 622381-40-2 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-[[4-(phenylmethyl)-1-piperazinyl]methyl]phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 622381-41-3 CAPLUS

2-Benzothiazoleacetonitrile, α-[2-[[4-[[4-(phenylmethyl)-1-piperazinyl]methyl]phenyl]methoxyl-4-pyrimidinyl]-, dimethanesulfonate (9CI) (CA INDEX NAME)

CM 1

CN

CRN 622381-40-2

CMF C32 H30 N6 O S

CM 2

CRN 75-75-2 CMF C H4 O3 S

RN 622381-42-4 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[4-[(4-ethyl-1-piperazinyl)methyl]phenyl]methoxy]- (9CI) (CA INDEX NAME)

RN 622381-43-5 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[4-[[4-(2-methoxyethyl)-1-piperazinyl]methyl]phenyl]methoxy]- (9CI) (CA INDEX NAME)

PAGE 1-B

— оме

RN 622381-44-6 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[4-[[4-(2-methoxyethyl)-1-piperazinyl]methyl]phenyl]methoxy]-, tris(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 622381-43-5 CMF C28 H30 N6 O2 S

PAGE 1-A
CH2-CH2-CH2
NH
O-CH2-N

PAGE 1-B

— оме

CM :

CRN 76-05-1 CMF C2 H F3 O2

RN 622381-45-7 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-(1-

piperazinylmethyl)phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 622381-46-8 CAPLUS

CN 2-Benzothiazoleacetonitrile, α -[2-[[4-(1-

piperazinylmethyl)phenyl]methoxy]-4-pyrimidinyl]-, tris(trifluoroacetate)
(9CI) (CA INDEX NAME)

CM :

CRN 622381-45-7

CMF C25 H24 N6 O S

CM 2

CRN 76-05-1

CMF C2 H F3 O2

RN 622381-47-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, \(\alpha = \frac{1}{2} - \left[(4-\frac{1}{4} - \frac{1}{4} - \fra

RN 622381-48-0 CAPLUS

CN 2-Benzothiazoleacetonitrile, α=[2-[[4-[4-formyl-1piperazinyl]methyl]phenyl]methoxyl-4-pyrimidinyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM

CRN 622381-47-9 CMF C26 H24 N6 O2 S

CM :

CRN 76-05-1 CMF C2 H F3 O2

RN 622381-49-1 CAPLUS

CN Piperazine, 1-(aminoacetyl)-4-[[4-[[4-(2(3H)-benzothiazolylidenecyanomethyl)-2-pyrimidinyl]oxy]methyl]phenyl]methyl](9C1) (CA INDEX NAME)

RN 622381-50-4 CAPLUS

Piperazine, 1-(aminoacetyl)-4-[[4-[[4-(2(3H)-benzothiazolylidenecyanomethyl)-2-pyrimidinyl)coxy]methyl]phenyl]methyl]-, dimethanesulfonate tris(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CN

CRN 622381-49-1 CMF C27 H27 N7 O2 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

F-C-CO2H

CM 3

CRN 75-75-2 CMF C H4 O3 S

RN 622381-51-5 CAPLUS

CN Piperazine, 1-acetyl-4-[[4-[[4-(2-benzothiazolylcyanomethyl)-2-pyrimidinyl]oxy]methyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 622381-52-6 CAPLUS

CN Piperazine, 1-acetyl-4-[[4-[[4-(2-benzothiazolylcyanomethyl)-2-pyrimidinyl]oxy]methyl]phenyl]methyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM

CRN 622381-51-5

CMF C27 H26 N6 O2 S

CM 2

CRN 76-05-1

CMF C2 H F3 O2

RN 622381-53-7 CAPLUS

CN 1-Piperazinecarboxamide, 4-[[4-[[[4-(2(3H)-benzothiazolylidenecyanomethyl)-

2-pyrimidinyl]oxy]methyl]phenyl]methyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)

RN 622381-54-8 CAPLUS

CN 1-Piperazinecarboxamide, 4-[[4-[2(3H)-benzothiazolylidenecyanomethyl)-2-pyzimidinyl]oxy]methyl]phenyl]methyl]-n,N-dimethyl-,bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 622381-53-7

CMF C28 H29 N7 O2 S

CM 2

CRN 76-05-1

CMF C2 H F3 O2

RN 622381-55-9 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[4-[[4-(2(3H)-benzothiazolylidenecyanomethyl)-2-pyrimidinyl]oxy]methyl]phenyl]methyl]-, methyl ester (9C1) (CA INDEX NAME)

RN 622381-56-0 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[4-[[[4-(2(3H)-benzothiazolylidenecyanomethyl]-2-pyrimidinyl]oxy]methyl]phenyl]methyl]-, methyl ester, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM

CRN 622381-55-9 CMF C27 H26 N6 O3 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 622381-57-1 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[4-[[4-(1,2,4-oxadiazol-3-ylmethyl)-1-piperazinyl]methyl]phenyl]methoxy]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

RN 622381-58-2 CAPLUS CN

d2330-30-2 ΔF103 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[{4-[[4-(1,2,4-oxadiazol-3-ylmethyl)-1-piperazinyl]methyl]phenyl]methoxy]-, tris(trifluoroacetate) (9CI) (CA INDEX MAME)

CM 1

CRN 622381-57-1 CMF C28 H26 N8 O2 S

PAGE 1-A

PAGE 1-B

CRN 76-05-1 CMF C2 H F3 O2

RN 622381-59-3 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[4-[[4-(2-hydroxyethyl)-1-piperazinyl]methyl]phenyl]methoxy]- (9CI) (CA INDEX NAME)

RN 622381-60-6 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[4-[[4-(2-hydroxyethyl)-1-piperazinyl]methyl]phenyl]methoxy)-, tris(trifluoroacetate) (salt) (9C1) (CA INDEX NAME)

CM 1

CRN 622381-59-3

CMF C27 H28 N6 O2 S

CM 2

CRN 76-05-1

CMF C2 H F3 O2

RN 622381-61-7 CAPLUS

CN 1-Piperazineacetic acid, 4-[[4-(2(3H)-benzothiazolylidenecyanomethyl)-

2-pyrimidinyl]oxy]methyl]phenyl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 622381-62-8 CAPLUS

CN 1-Piperazineacetic acid, 4-[[4-[[4-(2(3H)-benzothiazolylidenecyanomethyl)-2-pyrimidinyl]oxy]methyl]phenyl]methyl]-, methyl ester, tris(trifluoroacetate) (9CI) (CA INDEX NAME)

CM '

CRN 622381-61-7 CMF C28 H28 N6 O3 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 622381-63-9 CAPLUS

CN 1-Piperazineacetamide, 4-[[4-[[4-(2(3H)-benzothiazolylidenecyanomethyl)-2-pyrimidinyl]oxy]methyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 622381-64-0 CAPLUS

CN 1-Piperazineacetamide, 4-[[4-[[4-(2(3H)-benzothiazolylidenecyanomethyl)-2-pyrlmidinyl]oxy]methyl]phenyl]methyl]-, tris(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 622381-63-9 CMF C27 H27 N7 O2 S

CM :

CRN 76-05-1 CMF C2 H F3 O2

IT 345986-38-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of piperazine benzothiazoles as inhibitors of JNK kinases) RN 345986-38-1 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-(2-chloro-4-pyrimidinyl)- (9CI) (CA INDEX NAME)

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 14 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN

T.4

```
AΝ
     2003:454111 CAPLUS
DN
     139:36533
TΙ
     Benzazole derivatives for the treatment of scleroderma
ΤN
     Gotteland, Jean-Pierre; Gaillard, Pascale; Chyatchko, Yolande
PA
     Applied Research Systems ARS Holding N.V., Neth.
     PCT Int. Appl., 44 pp.
so
     CODEN: PIXXD2
חידים
     Patent
LA
     English
FAN.CNT 1
     PATENT NO.
                         KIND
                                 DATE
                                             APPLICATION NO.
                                                                  DATE
     WO 2003047570
                                 20030612
PT
                          A1
                                              WO 2002-EP13857
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ,
             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     CA 2468826
                                 20030612 CA 2002-2468826
                           AA
                                                                       20021206
     AU 2002352227
                                             AU 2002-352227
                           A1
                                 20030617
                                                                       20021206
     EP 1450792
                                             EP 2002-787919
                           A1
                                 20040901
                                                                       20021206
     EP 1450792
                           В1
                                 20060927
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK
     JP 2005515994
                           T2
                                 20050602
                                              JP 2003-548825
                                                                      20021206
     US 2005119277
                           A1
                                 20050602
                                              US 2003-496785
                                                                      20021206
PRAI EP 2001-727
                                 20011207
                           Α
     WO 2002-EP13857
                                 20021206
                           W
OS
     MARPAT 139:36533
ΔR
     The present invention is related to the use of benzazole derivs. I [X = 0,
     etc.; G = pyrimidinyl; R1 = H, alkoxy, etc.; R2 = H, alkyl, etc.] for the treatment and/or prevention of scleroderma and its therapeutic
     implications selected in the group consisting of systemic sclerosis.
     scleroderma-like disorders, liver cirrhosis, interstitial pulmonary
     fibrosis, Dupuytren's contracture, keloid and other scarring/wound healing
     abnormalities, postoperative adhesions, etc. The bioactivities of one compound of this invention were demonstrated. Formulations are given.
TΤ
     541507-15-7P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (preparation of benzazole derivs. for treatment of scleroderma)
RN
     541507-15-7 CAPLUS
CN
     4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[4-(4-
     morpholinylmethyl)phenyllmethoxyl-, mono(trifluoroacetate) (9CI) (CA
     INDEX NAME)
     CM
     CRN 541507-14-6
     CMF C25 H23 N5 O2 S
```

CM 2

CRN 76-05-1 CMF C2 H F3 O2

IT 541507-19-1 RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of benzazole derivs. for treatment of scleroderma) RN 541507-19-1 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-chloro-(9CI) (CA INDEX NAME)

IT 541507-14-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of benzazole derivs. for treatment of scleroderma)

(preparation of benzazole derivs. for t RN 541507-14-6 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[4-(4-morpholinylmethyl)phenyl]methoxy]- (9CI) (CA INDEX NAME)

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 15 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2002:502303 CAPLUS

DN 138:24685

TI Reaction of 2-hetarylacetonitriles with ethyl 2-alkylsulfanyl-4-chloro-5pyrimidinecarboxylates. Synthesis of new condensed pyrimidines

AU Blyumin, E. V.; Volovenko, Yu. M.; Neunhoeffer, Hans; Shishkina, S. V.; Zubatyuk, R. A.; Shishkin, Oleg V.

CS Chemical Department, Kiev Taras Schevchenko University, Kiev, 01033,

SO Tetrahedron (2002), 58(28), 5733-5740

CODEN: TETRAB; ISSN: 0040-4020

PB Elsevier Science Ltd.

DT Journal

LA English

OS CASREACT 138:24685

AB Reactions of 2-hetarylacetonitriles RICH2CN (I) (R1 = 2-pyridy),
2-benzimidazolyl, 1-methyl-2-benzimidazolyl, 2-benzothiazolyl) with Et
2-alkylsulfanyl-4-chloro-5-pyrimidinecarboxylates II (R2 = Me, PhCH2)
afforded a series of new condensed pyridopyrimidines, e.g. III. On the
other hand, the analogous reaction of benzoxazole and 4-arylthiazole
derived I, e.g. IV (R3 = Me3C, 4-ClCGH4, 4-BrCGH4), gave
4-[(2-hetaryl)-cyano-methyl]-2-alkylsulfanylpyrimidine-5-carboxylates,
e.g. V. Reactions of quinazoline derived I initially afforded stable
intermediate similar to V which on heating with K2CO3 formed the angular
polycyclic compound VI. The influence of the basicity of heterocycles and
of steric factors on the intramol. acylation reaction was studied.
IT 47879-90-6F

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (heteroaryl)pyrimidineacetonitriles and condensed
pyridopyrimidines via condensation of heteroaryl acetonitriles with
alkylthio(chloro)pyrimidinecarboxylates)

RN 477879-90-6 CAPLUS

CN

5-Pyrimidinecarboxylic acid, 4-(2-benzothiazolylcyanomethyl)-2-(methylthio)-, ethyl ester (9CI) (CA INDEX NAME)

RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2001:472001 CAPLUS
- DN 135:61322
- TI Preparation of benzazole derivatives as JNK modulators
- IN Halazy, Serge; Church, Dennis; Camps, Montserrat; Gaillard, Pascale; Gotteland, Jean-Pierre
- PA Applied Research Systems Ars Holding N.V., Neth. Antilles
- SO Eur. Pat. Appl., 31 pp.
- CODEN: EPXXDW
- DT Patent
- LA English

FAN.CNT 1																		
	PATENT NO. KI						DATE			APPLICATION NO.						DATE		
PI		EP 1110957								EP 1999-811207								
		R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR	, IT,	LI,	LU,	NL,	SE,	MC,	PT,
			IE,	SI,	LT,	LV,	FI,	RO										
									CA 2000-2394809									
	WO	2001047920				A1					WO 2000-EP13006							
		W:										, BG,						
												, FI,						
												, KR,						
												, MZ,						
						SI,	SK,	SL,	ТJ,	TM,	TR	, TŤ,	TZ,	UA,	UG,	US,	UZ,	VN,
				ZA,														
		RW:										, TZ,						
												, LU,						BF,
												, MR,						
	EP	1240164				A1		2002	EP 2000-991229					20001220				
	EΡ	1240164 R: AT, BE,				B1		2003										
		R:											LI,	LU,	NL,	SE,	MC,	PT,
												, TR				_		
	TR	200201509				T2		2002	TR 2002-1509						20001220			
	BR	2000016911				A		2002	BR 2000-16911						20001220			
	J.F	2003	2131		12		2003	JP 2001-549390 EE 2002-318 AT 2000-991229 PT 2000-991229 NZ 2000-519423				20001220						
	EE	2002		A		2003	EE 2002-318				20001220							
	AT	234123				- E		2003		MI 2000-991229				20001220				
	PI	124U104				T		2004	NT 2000-991229					20001220				
	NZ	2206351				A.		2004		NZ 2000-319423 ES 2000-991229					20001220			
		780241						2004	AU 2001-21616									
	77	200241				7		2003		ZA 2002-4427					20001220			
	DC.	106830				Α.		2004		ZA 2002-14427 BG 2002-106830 NO 2002-2997					20020603			
	NO.	2002002007				^		2003		NO 2002-100030					20020621			
	IIS	2002002337				A1		2002		US 2002-2997								
	03	2003	1021	74		WI		2003		03 2002-100710					20021021			

HK 1055730 PRAI EP 1999-811207 WO 2000-EP13006 OS MARPAT 135:61322

OS PARKAI 153:01522

AB The title compds. [I: X = O, S, NRO; G = (un)substituted aryl, heteroaryl, 3-8-membered (un)saturated ring system containing at least one heteroatom selected

20060728

19991224 20001220

A1

Α.

from N, O or S (said 3-8-membered ring system may be fused with (un)substituted aryl or heteroaryl system thus providing a bicyclic system); R1 = H, alkoxy, thioalkoxy, etc.; R2 = H, alkyl, alkenyl, etc.] which are efficient modulators of the JNK pathway, in particular efficient and selective inhibitors of JNK2 and/or 3, were prepared and formulated. E.g., a 2-step synthesis of I [X = S; R1, R2 = H; G = 2-[2-(1H-imidazol-4-E.g., a 2-step synthesis of I [X = S; R1, R2 = H; G = 2-[2-(1H-imidazol-4-E.g., a 2-step synthesis of I [X = S; R1, R2 = H; G = 2-[2-(1H-imidazol-4-E.g., a 2-step synthesis of I [X = S; R1, R2 = H; G = 2-[2-(1H-imidazol-4-E.g., a 2-step synthesis of I [X = S; R1, R2 = H; G = 2-[2-(1H-imidazol-4-E.g., a 2-step synthesis of I [X = S; R1, R2 = H; G = 2-[2-(1H-imidazol-4-E.g., a 2-step synthesis of I [X = S; R1, R2 = H; G = 2-[2-(1H-imidazol-4-E.g., a 2-step synthesis of I [X = S; R1, R2 = H; G = 2-[2-(1H-imidazol-4-E.g., a 2-step synthesis of I [X = S; R1, R2 = H; G = 2-[2-(1H-imidazol-4-E.g., a 2-step synthesis of I [X = S; R1, R2 = H; G = 2-[2-(1H-imidazol-4-E.g., a 2-step synthesis of I [X = S; R1, R2 = H; G = 2-[2-(1H-imidazol-4-E.g., a 2-step synthesis of I [X = S; R1, R2 = H; G = 2-[2-(1H-imidazol-4-E.g., a 2-step synthesis of I [X = S; R1, R2 = H; G = 2-[2-(1H-imidazol-4-E.g., a 2-step synthesis of I [X = S; R1, R2 = H; G = 2-[2-(1H-imidazol-4-E.g., a 2-step synthesis of I [X = S; R1, R2 = H; G = 2-[2-(1H-imidazol-4-E.g., a 2-step synthesis of I [X = S; R1, R2 = H; G = 2-[2-(1H-imidazol-4-E.g., a 2-step synthesis of I [X = S; R1, R2 = H; G = 2-[2-(1H-imidazol-4-E.g., a 2-step synthesis of I [X = S; R1, R2 = H; G = 2-[2-(1H-imidazol-4-E.g., a 2-step synthesis of I [X = S; R1, R2 = H; G = 2-[2-(1H-imidazol-4-E.g., a 2-step synthesis of I [X = S; R1, R2 = H; G = 2-[2-(1H-imidazol-4-E.g., a 2-step synthesis of I [X = S; R1, R2 = H; G = 2-[2-(1H-imidazol-4-E.g., a 2-step synthesis of I [X = S; R1, R2 = H; G = 2-[2-(1H-imidazol-4-E.g., a 2-step synthesis of I [X = S; R1, A] [X = H; G = 2-[2-(1

нк 2003-107978

20031105

10/511,438

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yl)ethylamino]-4-pyrimidinyl] which showed IC50 of 70 nM and of 210 nM
     against JNK3 and JNK2, resp., was given.
TТ
     345986-38-1P 345986-40-5P 345986-44-9P
     345986-46-1P 345986-48-3P 345986-50-7P
     345986-64-3P 345986-65-4P 345986-66-5P
     345986-67-6P 345986-69-8P 345986-70-1P
     345986-72-3P 345986-73-4P 345986-75-6P
     345986-76-7P 345986-78-9P 345986-79-0P
     345986-81-4P 345986-82-5P 345986-84-7P
     345986-85-8P 345986-86-9P 345986-87-0P
     345986-88-1P 345986-89-2P 345986-91-6P
     345986-92-7P 345986-94-9P 345986-96-1P
     345986-98-3P 345986-99-4P 345987-00-0P
     345987-01-1P 345987-02-2P 345987-03-3P
     345987-04-4P 345987-05-5P 345987-06-6P
     345987-07-7P 345987-09-9P 345987-10-2P
     345987-11-3P 345987-12-4P 345987-13-5P
     345987-14-6P 345987-15-7P 345987-16-8P
     345987-17-9P 345987-19-1P 345987-20-4P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of benzazole derivs. as JNK modulators)
RN
     345986-38-1 CAPLUS
CN
     2-Benzothiazoleacetonitrile, \alpha-(2-chloro-4-pyrimidinyl)- (9CI) (CA
```

INDEX NAME)

RN 345986-40-5 CAPLUS

CN

CN

2-Benzothiazoleacetonitrile, α -(2,6-dimethoxy-4-pyrimidinyl)- (9CI) (CA INDEX NAME)

RN 345986-44-9 CAPLUS

2-Benzothiazoleacetonitrile, α -(2-chloro-6-methyl-4-pyrimidinyl)-(9CI) (CA INDEX NAME)

RN 345986-46-1 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-(methylthio)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 345986-48-3 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-(6-chloro-5-nitro-4-pyrimidinyl)-(9CI) (CA INDEX NAME)

RN 345986-50-7 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-2-pyrimidinyl- (9CI) (CA INDEX NAME)

RN 345986-64-3 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(1H-imidazol-4-yl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

10/511.438

RN 345986-65-4 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(1H-imidazol-4-yl)ethyl]amino]-4-pyrimidinyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 345986-64-3 CMF C18 H15 N7 S

CM .

CRN 76-05-1 CMF C2 H F3 O2

RN 345986-66-5 CAPLUS CN 2-Benzothiazoleacetonitrile, α-[2-(1-piperaziny1)-4-pyrimidiny1]-(9C1) (CA INDEX NAME)

RN 345986-67-6 CAPLUS
CN 2-Benzothiazoleacetonitrile, \(\alpha - [2-(1-piperazinyl) - 4-pyrimidinyl] - \)
bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 345986-66-5 CMF C17 H16 N6 S

CM :

CRN 76-05-1

CMF C2 H F3 O2

RN 345986-69-8 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[4-(phenylmethyl)-1-piperidinyl]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 345986-70-1 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[4-(phenylmethyl)-1-piperidinyl]-4-pyrimidinyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 345986-69-8

CMF C25 H23 N5 S

CM 2

CRN 76-05-1

CMF C2 H F3 O2

RN 345986-72-3 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-(4-methyl-1-piperazinyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 345986-73-4 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-(4-methyl-1-piperazinyl)-4-pyrimidinyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM

CRN 345986-72-3 CMF C18 H18 N6 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 345986-75-6 CAPLUS

CN 2-Benzothiazoleacetonitrile, α -[2-(4-morpholiny1)-4-pyrimidiny1]-(9CI) (CA INDEX NAME)

RN 345986-76-7 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-(4-morpholinyl)-4-pyrimidinyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM

CRN 345986-75-6 CMF C17 H15 N5 O S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 345986-78-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, α -[2-(methylamino)-4-pyrimidinyl]-(9CI) (CA INDEX NAME)

RN 345986-79-0 CAPLUS

2-Benzothiazoleacetonitrile, α-[2-(methylamino)-4-pyrimidinyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CN

CRN 345986-78-9

CMF C14 H11 N5 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 345986-81-4 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[4-[2-(4-morpholinyl)ethyl]-1-piperazinyl]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 345986-82-5 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[4-[2-(4-morpholiny1)ethy1]-1-piperaziny1]-4-pyrimidiny1]-, tris(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 345986-81-4 CMF C23 H27 N7 O S

CM 2

RN 345986-84-7 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[4-(phenylmethoxy)-1-piperidinyl]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 345986-85-8 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[4-(phenylmethoxy)-1-piperidinyl]-4-pyrimidinyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM

CRN 345986-84-7 CMF C25 H23 N5 O S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 345986-86-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-(4-hydroxy-1-piperidinyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 345986-87-0 CAPLUS

N 2-Benzothiazoleacetonitrile, α-[2-(4-hydroxy-1-piperidinyl)-4-pyrimidinyl]-, mono(trifluoroacetate) (salt) (SCI) (CA INDEX NAME)

CM

CRN 345986-86-9 CMF C18 H17 N5 O S

CM

CRN 76-05-1 CMF C2 H F3 O2

RN 345986-88-1 CAPLUS

CN 2-Benzothiazoleacetonitrile, α -(2-hydrazino-4-pyrimidinyl)- (9CI) (CA INDEX NAME)

RN 345986-89-2 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-(2-hydrazino-4-pyrimidinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 345986-88-1 CMF C13 H10 N6 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 345986-91-6 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(dimethylamino)ethyl]amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 345986-92-7 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(dimethylamino)ethyl]amino]-4-pyrimidinyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 345986-91-6 CMF C17 H18 N6 S

CM 2

CRN 76-05-1

CMF C2 H F3 O2

RN 345986-94-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-(dimethylamino)-4-pyrimidinyl]-(9CI) (CA INDEX NAME)

RN 345986-96-1 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(2-methoxyethyl)amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 345986-98-3 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(2-hydroxyethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{CN} & \text{N} \\ & \text{CH} & \text{N} \\ & \text{NH-CH}_2\text{-CH}_2\text{-OH} \end{array}$$

RN 345986-99-4 CAPLUS

CN 2-Benzothiazoleacetonitrile, α -[2-(propylamino)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 345987-00-0 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[3-(1H-imidazol-1-yl)propyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 345987-01-1 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[3-(1H-imidazol-1-yl)propyl]amino]-4-pyrimidinyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 345987-00-0

CRN 345987-00-0 CMF C19 H17 N7 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 345987-02-2 CAPLUS

CN 2-Benzothiazoleacetonitrile, α -[2-(1-pyrrolidinyl)-4-pyrimidinyl]-(9CI) (CA INDEX NAME)

RN 345987-03-3 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(2-phenylethyl)amino]-4-

pyrimidinyl] - (9CI) (CA INDEX NAME)

RN 345987-04-4 CAPLUS

CN 2-Benzothiazoleacetonitrile, α -[2-[[2-(2-pyridinyl)ethyl]amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 345987-05-5 CAPLUS

CN 2-Benzothiazoleacetonitrile, α -[2-[[2-(2-pyridinyl)ethyl]amino]-4pyrimidinyl]-, bis(trifluoroacetate) (9CI) (CA ÎNDEX NAME)

CM

CRN 345987-04-4 CMF C20 H16 N6 S

CM

CRN 76-05-1

CMF C2 H F3 O2

RN 345987-06-6 CAPLUS

CN 2-Benzothiazoleacetonitrile, α -[2-[(2-pyridinylmethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 345987-07-7 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(2-pyridinylmethyl)amino]-4-pyrimidinyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 345987-06-6

CMF C19 H14 N6 S

CM 2

CRN 76-05-1

CMF C2 H F3 O2

RN 345987-09-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[4-(1H-benzotriazol-l-yl)-l-piperidinyl]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 345987-10-2 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[4-(1H-benzotriazol-1-yl)-1-piperidinyl]-4-pyrimidinyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 345987-09-9

CMF C24 H20 N8 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 345987-11-3 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-(4-pyrazinyl-1-piperazinyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 345987-12-4 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-(4-pyrazinyl-1-piperazinyl)-4-pyrimidinyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM

CRN 345987-11-3 CMF C21 H18 N8 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 345987-13-5 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[4-(2-pyrimidinyl)-1-piperazinyl]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 345987-14-6 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[4-(2-pyrimidinyl)-1-piperazinyl]-4-pyrimidinyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 345987-13-5 CMF C21 H18 N8 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 345987-15-7 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(3-pyridinyl)ethyl]amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 345987-16-8 CAPLUS

CN 2-Benzothiazoleacetonitrile, α -[2-[[2-(3-pyridinyl)ethyl]amino]-4-pyrimidinyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM

CRN 345987-15-7

CMF C20 H16 N6 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 345987-17-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[5-bromo-2-[[2-(dimethylamino)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 345987-19-1 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-(2-methoxy-4-pyrimidinyl)- (9CI) (CA INDEX NAME)

RN 345987-20-4 CAPLUS

CN 4-Pyrimidineacetonitrile, 2-chloro-α-(3-methyl-2(3H)-benzothiazolylidene)- (9CI) (CA INDEX NAME)

RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT